

# A description of the Hubbard model on a square lattice consistent with its global $SO(3) \times SO(3) \times U(1)$ symmetry

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In this paper a description of the Hubbard model on the square lattice with nearest-neighbor transfer integral  $t$ , on-site repulsion  $U$ , and  $N_a^2 \gg 1$  sites consistent with its exact global  $SO(3) \times SO(3) \times U(1)$  symmetry is constructed. Our studies profit from the interplay of that recently found global symmetry of the model on any bipartite lattice with the transformation laws under a suitable electron - rotated-electron unitary transformation of a well-defined set of operators and quantum objects. For  $U/4t > 0$  the occupancy configurations of these objects generate the energy eigenstates that span the one- and two-electron subspace. Such a subspace as defined in this paper contains nearly the whole spectral weight of the excitations generated by application onto the zero-spin-density ground state of one- and two-electron operators. Our description involves three basic objects: charge  $c$  fermions, spin-1/2 spinons, and  $\eta$ -spin-1/2  $\eta$ -spinons. Independent spinons and independent  $\eta$ -spinons are invariant under the above unitary transformation. Alike in chromodynamics the quarks have color but all quark-composite physical particles are color-neutral, the  $\eta$ -spinon (and spinons) that are not invariant under that transformation have  $\eta$  spin 1/2 (and spin 1/2) but are part of  $\eta$ -spin-neutral (and spin-neutral)  $2\nu$ - $\eta$ -spinon (and  $2\nu$ -spinon) composite  $\eta\nu$  fermions (and  $s\nu$  fermions) where  $\nu = 1, 2, \dots$  is the number of  $\eta$ -spinon (and spinon) pairs. The occupancy configurations of the  $c$  fermions, independent spinons and  $2\nu$ -spinon composite  $s\nu$  fermions, and independent  $\eta$ -spinons and  $2\nu$ - $\eta$ -spinon composite  $\eta\nu$  fermions correspond to the state representations of the  $U(1)$ , spin  $SU(2)$ , and  $\eta$ -spin  $SU(2)$  symmetries, respectively, associated with the model  $SO(3) \times SO(3) \times U(1) = [SU(2) \times SU(2) \times U(1)]/Z_2^2$  global symmetry. The components of the  $\alpha\nu$  fermion discrete momentum values  $\vec{q}_j = [q_{j\,x1}, q_{j\,x2}]$  are eigenvalues of the corresponding set of  $\alpha\nu$  translation generators in the presence of fictitious magnetic fields  $\vec{B}_{\alpha\nu}$ . Our operator description has been constructed to inherently the  $\alpha\nu$  translation generators  $\vec{q}_{\alpha\nu}$  in the presence of the fictitious magnetic field  $\vec{B}_{\alpha\nu}$  commuting with the momentum operator, consistently with their component operators  $\hat{q}_{\alpha\nu\,x1}$  and  $\hat{q}_{\alpha\nu\,x2}$  commuting with each other. In turn, unlike for the 1D model such generators not commute in general with the Hamiltonian, except for the Hubbard model on the square lattice in the one- and two-electron subspace. Concerning one- and two-electron excitations, the picture that emerges is that of a two-component quantum liquid of charge  $c$  fermions and spin-neutral two-spinon  $s1$  fermions. The description introduced here is consistent with a Mott-Hubbard insulating ground state with antiferromagnetic long-range order for half filling at  $x = 0$  hole concentration and a ground state with short-range spin order for a well-defined range of finite hole concentrations  $x > 0$ . For  $0 < x \ll 1$  the latter short-range spin order has an incommensurate-spiral character. Our results are of interest for studies of ultra-cold fermionic atoms on optical lattices and elsewhere evidence is provided that upon addition of a small three-dimensional anisotropy plane-coupling perturbation to the square-lattice quantum liquid considered here its short-range spin order coexists for low temperatures and a well-defined range of hole concentrations with a long-range superconducting order so that the use of the general description introduced in this paper contributes to the further understanding of the role of electronic correlations in the unusual properties of the hole-doped cuprates.

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## I. INTRODUCTION

There is some consensus that the Hubbard model on a square lattice is the simplest toy model for describing the effects of electronics correlations in high- $T_c$  superconductors<sup>1-6</sup> and their Mott-Hubbard insulators parent compounds<sup>7</sup>. In addition, the model can be experimentally realized with unprecedented precision in systems of ultra-cold fermionic atoms on an optical lattice and one may expect very detailed experimental results over a wide range of parameters to be available<sup>8</sup>. That includes recent studies on systems of ultra-cold fermionic atoms describing the Mott-Hubbard insulating phase of the the Hubbard model on a cubic lattice<sup>9</sup>. Unfortunately, the model has no exact solution and many open questions about its properties remain unsolved. A recent exact result, which applies to the model on any bipartite lattice<sup>2</sup>, is that for on-site repulsion  $U > 0$  its global symmetry is  $SO(3) \times SO(3) \times U(1) = [SO(4) \times U(1)]/Z_2$ . That is an extension of the model well-known  $SO(4)$  symmetry<sup>10</sup>, which becomes explicit provided that one describes the problem in terms of the rotated electrons obtained from the electrons by any of the unitary transformations of the type considered in Refs.<sup>2,11</sup>.

In this paper a general description is introduced for the Hubbard model on the two-dimensional (2D) square lattice with spacing  $a$ ,  $N_a^D \equiv [N_a]^D$  sites,  $D = 2$ ,  $N_a$  even, and lattice edge length  $L = N_a a$ . (Due to editorial decisions, the results presented in this paper were distributed over three articles, specifically Refs.<sup>2-4</sup>. We thus forward the reader to these references, in which the presentation of the results was further improved, yet the scientific message remains the same.)

The representation introduced here refers to suitable quantum objects whose occupancy configurations generate the state representations of the group  $SO(3) \times SO(3) \times U(1)$ . Addition of chemical-potential and magnetic-field operator terms to the Hamiltonian lowers its symmetry. Such terms commute though with it and the momentum and energy eigenstates correspond to representations of that group. It is shown in Appendix A that all the physics of the model in the whole Hilbert space can be obtained from that of the model in the subspace spanned by the lowest-weight states (LWSs) of both the  $\eta$ -spin  $SU(2)$  and spin  $SU(2)$  algebras. Hence often our results refer to that large subspace. Another subspace that plays a key role in our description is the one- and two-electron subspace defined in Section V. For 2D, the states generated by the momentum occupancy configurations of the above objects belonging to such a subspace are for  $U/4t > 0$  energy eigenstates.

Furthermore, often we discuss the use of our description for the model on an one-dimensional (1D) lattice as well, so that the coefficient  $D$  appearing in several quantities considered in this paper may have the values  $D = 1, 2$ . Due to the integrability of the 1D model, the states generated by the momentum occupancy configurations of the above-mentioned objects are exact energy eigenstates for the whole Hilbert space and all values of  $U/4t$ . Our results refer to a very large system whose lattice has  $N_a^D \gg 1$  sites and for the square (and 1D) lattice torus periodic boundary conditions (and periodic boundary conditions) are used. The description involves the generalization to all finite values of the on-site repulsion  $U > 0$  of the exact transformation for separation of spin-1/2 fermions without constraints introduced for large  $U$  values in Ref.<sup>12</sup>.

The global  $SO(3) \times SO(3) \times U(1)$  symmetry refers to the Hubbard model on any bipartite lattice. Hence it applies to the  $D$ -dimensional cubic lattice<sup>13,14</sup>. However, some of the results obtained below are valid for the square lattice only. In spite of our study focusing onto the model on that lattice, the reason why often our analysis refers to the corresponding 1D problem as well is that in contrast to real-space dimensions  $D > 1$  there is an exact solution for the model on a 1D lattice<sup>15-17</sup>. Our quantum-object description also applies to 1D, yet due to the integrability of the model often it then leads to a different physics. In turn, one of the procedures used to control the validity of the approximations used in the construction of our description profits both from identifying the common proprieties of the model on the square and 1D lattices and checking whether they are valid for the model on the latter lattice by means of its exact solution. Some of these common properties are related to the model commuting with the generators of the group  $SO(3) \times SO(3) \times U(1)$  both for the square and 1D bipartite lattices.

For such two lattices the fulfillment of our program reveals the emergence of three basic quantum objects: spin-less and  $\eta$ -spin-less charge  $c$  fermions, spin-1/2 spinons, and  $\eta$ -spin-1/2  $\eta$ -spinons. In principle there are some occupancy configurations of such objects that generate the exact momentum and energy eigenstates for  $U/4t > 0$ , yet the detailed structure of such configurations is a complex problem. It simplifies in the one- and two-electron subspace constructed in this paper, where for the model on the square lattice and  $U/4t > 0$  the occupancy configurations of the above objects generate exact ground states and excited energy eigenstates. Such a subspace contains nearly the whole spectral weight generated by application onto the zero-spin-density ground state of one- and two-electron operators. Throughout this paper we often call that subspace *one- and two-electron subspace*. In reference<sup>18</sup> the spinon occupancy configurations of the states that span that subspace are studied.

The composite  $2\nu$ - $\eta$ -spinon  $\eta\nu$  fermions (and  $2\nu$ -spinon  $s\nu$  fermions) emerge from  $\eta$ -spin (and spin) neutral  $\eta\nu$  bond particles (and  $s\nu$  bond particles) through extended Jordan-Wigner transformations<sup>19-21</sup>. For the model on the square lattice the two-spinon  $s1$  bond particles are found in Refs.<sup>1,22</sup> to be closely related to the spin-singlet bonds of Ref.<sup>23</sup>. It is confirmed in Appendix B that for 1D the discrete momentum values of the  $c$  fermions and  $\alpha\nu$  fermions are good quantum numbers for all  $U/4t$  values and their momentum occupancy configurations generate the exact energy eigenstates. Evidence that for the one- and two-electron subspace the states generated by the occupancy configurations of such discrete momentum values are for the model on the square lattice and  $U/4t > 0$  energy eigenstates is given in this paper and in Ref.<sup>1</sup>.

The paper is organized as follows. The model, the uniquely defined rotated-electron description used in our studies, its limitations and usefulness, and the global  $SO(3) \times SO(3) \times U(1)$  symmetry are the subjects of Section II. In Section III the  $c$  fermion,  $\eta$ -spin-1/2  $\eta$ -spinon, and spin-1/2 spinon and corresponding  $c$ ,  $\eta$ -spin, and spin effective lattices are introduced. The vacua of the theory, their transformation laws under the electron - rotated-electron unitary transformation, and the subspaces they refer to are issues also addressed in that section. The composite  $\alpha\nu$  bond particles and  $\alpha\nu$  fermions, corresponding  $\alpha\nu$  effective lattices, ground-state occupancy configurations, and a suitable complete set of momentum eigenstates are the subjects of Section IV. In Section V the one- and two-electron subspace where only the  $c$  fermions and  $s1$  fermions play an active role is introduced. The corresponding  $c$  and  $s1$  effective lattices and elementary excitations are discussed. In Section VI it is shown that the description introduced in this

paper is consistent with a Mott-Hubbard insulating ground state with long-range antiferromagnetic order for half filling and a ground state with short-range spin order for a well-defined range of finite hole concentrations. Strong evidence is given that for  $0 < x \ll 1$  and intermediate and large values of  $U/4t$  the latter order has an incommensurate-spiral character. Section VII contains the concluding remarks. Moreover, that the whole physics can be extracted from the Hubbard model in the LWS subspace spanned by the  $\eta$ -spin and spin LWSs is confirmed in Appendix A. In Appendix B it is confirmed that the general operator description introduced in this paper for the Hubbard model on the square and 1D lattices is consistent with the exact solution of the 1D problem. For instance, it is confirmed that the discrete momentum values of the  $c$  fermions and composite  $\alpha\nu$  fermions are good quantum numbers. Furthermore, in that Appendix the relation of the creation and annihilation fields of the charge ABCDF algebra<sup>16</sup> and more traditional spin ABCD Faddeev-Zamolodchikov algebra<sup>24</sup> of the algebraic formulation of the 1D exact solution of Ref.<sup>16</sup> to the  $c$  and  $\alpha\nu$  fermion operators is discussed and the consistency between the two corresponding operational representations confirmed.

## II. THE MODEL, A SUITABLE ROTATED-ELECTRON DESCRIPTION, AND THE GLOBAL $SO(3) \times SO(3) \times U(1)$ SYMMETRY

### A. The model, a suitable rotated-electron description, and its limitations and usefulness

The Hubbard model is given by,

$$\hat{H} = t\hat{T} + U[N_a^D - \hat{Q}]/2; \quad \hat{T} = - \sum_{\langle \vec{r}_j \vec{r}_{j'} \rangle} \sum_{\sigma} [c_{\vec{r}_j, \sigma}^{\dagger} c_{\vec{r}_{j'}, \sigma} + h.c.]; \quad \hat{Q} = \sum_{j=1}^{N_a^D} \sum_{\sigma=\uparrow, \downarrow} n_{\vec{r}_j, \sigma} (1 - n_{\vec{r}_j, -\sigma}). \quad (1)$$

Here  $D = 1$  and  $D = 2$  for the 1D and square lattices, respectively,  $t$  is the nearest-neighbor transfer integral,  $\hat{T}$  the kinetic-energy operator in units of  $t$ ,  $\hat{Q}$  the operator that counts the number of electron singly occupied sites so that the operator  $\hat{D} = [\hat{N} - \hat{Q}]/2$  counts the number of electron doubly occupied sites,  $n_{\vec{r}_j, \sigma} = c_{\vec{r}_j, \sigma}^{\dagger} c_{\vec{r}_j, \sigma}$  where  $-\sigma = \uparrow$  (and  $-\sigma = \downarrow$ ) for  $\sigma = \downarrow$  (and  $\sigma = \uparrow$ ),  $\hat{N} = \sum_{\sigma} \hat{N}_{\sigma}$ , and  $\hat{N}_{\sigma} = \sum_{j=1}^{N_a^D} n_{\vec{r}_j, \sigma}$ . The kinetic-energy operator  $\hat{T}$  can be expressed in terms of the operators,

$$\begin{aligned} \hat{T}_0 &= - \sum_{\langle \vec{r}_j \vec{r}_{j'} \rangle} \sum_{\sigma} [n_{\vec{r}_j, -\sigma} c_{\vec{r}_j, \sigma}^{\dagger} c_{\vec{r}_{j'}, \sigma} n_{\vec{r}_{j'}, -\sigma} + (1 - n_{\vec{r}_j, -\sigma}) c_{\vec{r}_j, \sigma}^{\dagger} c_{\vec{r}_{j'}, \sigma} (1 - n_{\vec{r}_{j'}, -\sigma}) + h.c.], \\ \hat{T}_{+1} &= - \sum_{\langle \vec{r}_j \vec{r}_{j'} \rangle} \sum_{\sigma} [n_{\vec{r}_j, -\sigma} c_{\vec{r}_j, \sigma}^{\dagger} c_{\vec{r}_{j'}, \sigma} (1 - n_{\vec{r}_{j'}, -\sigma}) + h.c.], \\ \hat{T}_{-1} &= - \sum_{\langle \vec{r}_j \vec{r}_{j'} \rangle} \sum_{\sigma} [(1 - n_{\vec{r}_j, -\sigma}) c_{\vec{r}_j, \sigma}^{\dagger} c_{\vec{r}_{j'}, \sigma} n_{\vec{r}_{j'}, -\sigma} + h.c.], \end{aligned} \quad (2)$$

as  $\hat{T} = \hat{T}_0 + \hat{T}_{+1} + \hat{T}_{-1}$ . These three kinetic operators play an important role in the physics. The operator  $\hat{T}_0$  does not change electron double occupancy whereas the operators  $\hat{T}_{+1}$  and  $\hat{T}_{-1}$  do it by +1 and -1, respectively.

The studies of Ref.<sup>2</sup> consider unitary operators  $\hat{V} = \hat{V}(U/4t)$  and corresponding rotated-electron operators  $\hat{c}_{\vec{r}_j, \sigma}^{\dagger} = \hat{V}^{\dagger} c_{\vec{r}_j, \sigma}^{\dagger} \hat{V}$  such that rotated-electron single and double occupancy are good quantum numbers for  $U/4t > 0$ . The generator  $\hat{S}_c$  of the global  $U(1)$  symmetry given below and in that reference has eigenvalue  $S_c$  with  $2S_c$  being the number of rotated-electron singly occupied sites. Most choices of the unitary operators  $\hat{V}$  correspond to choices of  $U/4t \rightarrow \infty$  sets  $\{|\Psi_{\infty}\rangle\}$  of  $4^{N_a^D}$  energy eigenstates such that the states  $|\Psi_{U/4t}\rangle = \hat{V}^{\dagger} |\Psi_{\infty}\rangle$  are not energy and momentum eigenstates for finite  $U/4t$  values yet belong to a subspace with constant and well-defined values of  $S_c$ ,  $S_{\eta}$ , and  $S_s$ . Here  $S_{\eta}$  (and  $S_s$ ) denotes the  $\eta$ -spin (and spin) value of the energy eigenstates. We call  $S_{\eta}^z = -[N_a^D - N]/2$  (and  $S_s^z = -[N_{\uparrow} - N_{\downarrow}]/2$ ) the corresponding projection. We focus our attention on ground states with hole concentration  $x = [N_a^D - N]/N_a^D \geq 0$  and spin density  $m = [N_{\uparrow} - N_{\downarrow}]/N_a^D = 0$  and are particularly interested in the *LWS-subspace* spanned by the LWSs of both the  $\eta$ -spin and spin algebras. Such energy eigenstates refer to values of  $S_{\alpha}$  and  $S_{\alpha}^z$  such that  $S_{\alpha} = -S_{\alpha}^z$  for  $\alpha = \eta, s$ . Indeed, since the off-diagonal generators that generate the non-LWSs from the LWSs commute with the operator  $\hat{V}^2$ , the whole physics can be extracted from the model (1) in the LWS-subspace, as confirmed in Appendix A.

Let  $\{|\Psi_{U/4t}\rangle\}$  be a complete set of  $4^{N_a^D}$  energy, momentum,  $\eta$ -spin,  $\eta$ -spin projection, spin, and spin-projection eigenstates for  $U/4t > 0$ . In the limit  $U/4t \rightarrow \infty$  such states correspond to one of the many choices of sets  $\{|\Psi_{\infty}\rangle\}$

of  $4^{N_a^D} U/4t$ -infinite energy eigenstates. For this choice there exists exactly one unitary operator  $\hat{V} = \hat{V}(U/4t)$  such that  $|\Psi_{U/4t}\rangle = \hat{V}^\dagger |\Psi_\infty\rangle$ . Here we consider such a unitary operator and corresponding rotated-electron operators  $\tilde{c}_{\vec{r}_j, \sigma}^\dagger = \hat{V}^\dagger c_{\vec{r}_j, \sigma}^\dagger \hat{V}$ . The states  $|\Psi_{U/4t}\rangle = \hat{V}^\dagger |\Psi_\infty\rangle$  (one for each value of  $U/4t > 0$ ) that are generated from the same initial state  $|\Psi_\infty\rangle$  belong to the same  $V$  tower.

We associate with any operator  $\hat{O}$  a rotated operator  $\tilde{O} = \hat{V}^\dagger \hat{O} \hat{V}$  that has the same expression in terms of rotated-electron creation and annihilation operators as  $\hat{O}$  of electron creation and annihilation operators, respectively. Any operator  $\hat{O}$  can be written in terms of rotated-electron creation and annihilation operators as,

$$\begin{aligned} \hat{O} &= \hat{V} \tilde{O} \hat{V}^\dagger = \tilde{O} + [\tilde{O}, \hat{S}] + \frac{1}{2} [[\tilde{O}, \hat{S}], \hat{S}] + \dots = \tilde{O} + [\tilde{O}, \tilde{S}] + \frac{1}{2} [[\tilde{O}, \tilde{S}], \tilde{S}] + \dots, \\ \hat{S} &= \frac{t}{U} [\hat{T}_{+1} - \hat{T}_{-1}] + \mathcal{O}(t^2/U^2); \quad \tilde{S} = \frac{t}{U} [\tilde{T}_{+1} - \tilde{T}_{-1}] + \mathcal{O}(t^2/U^2). \end{aligned} \quad (3)$$

The operator  $\hat{S}$  appearing in this equation is related to the unitary operator as  $\hat{V}^\dagger = e^{\hat{S}}$  and  $\hat{V} = e^{-\hat{S}}$ . The general unknown expression of  $\hat{S}$  involves only the kinetic operators  $\hat{T}_0$ ,  $\hat{T}_{+1}$ , and  $\hat{T}_{-1}$  of Eq. (2) and numerical  $U/4t$  dependent coefficients and for  $U/4t > 0$  can be expanded in a series of  $t/U$ . The corresponding first-order term has the universal form given in Eq. (3). To arrive to the expression in terms of the operator  $\tilde{S}$  also given in Eq. (3), the property that the operator  $\hat{V}$  commutes with itself so that  $\hat{V} = e^{-\hat{S}} = \tilde{V} = e^{-\tilde{S}}$  and  $\hat{S} = \tilde{S}$  and both the operators  $\hat{V}$  and  $\tilde{S}$  have the same expression in terms of electron and rotated-electron creation and annihilation operators is used. This is behind the expansion  $\hat{S} = (t/U) [\hat{T}_{+1} - \hat{T}_{-1}] + \mathcal{O}(t^2/U^2)$  given in that equation for the operator  $\hat{S}$ . Its higher-order terms can be written as a product of operator factors whose expressions involve the rotated kinetic operators  $\tilde{T}_0$ ,  $\tilde{T}_{+1}$ , and  $\tilde{T}_{-1}$ . The full expression of the operator  $\hat{S} = \tilde{S}$  can for  $U/4t > 0$  be written as  $\hat{S} = \hat{S}(\infty) + \delta\hat{S} = \tilde{S}(\infty) + \delta\tilde{S}$  where  $\hat{S}(\infty) = \tilde{S}(\infty)$  corresponds to the operator  $S(l)$  at  $l = \infty$  defined in Eq. (61) of Ref.<sup>11</sup> and  $\delta\hat{S} = \delta\tilde{S}$  has the general form provided in its Eq. (64). The unitary operator  $\hat{V} = e^{-\hat{S}} = e^{-\tilde{S}}$  considered here corresponds to exactly one choice of the coefficients  $D^{(k)}(\mathbf{m})$  of that equation, where for the operator  $\tilde{V}$  the index  $k = 1, 2, \dots$  refers to the number of rotated-electron doubly occupied sites. The problem of finding the explicit form of the operators  $\hat{V} = \tilde{V}$  and  $\hat{S} = \tilde{S}$  is equivalent to finding all coefficients  $D^{(k)}(\mathbf{m})$  associated with the electron - rotated-electron unitary transformation as defined in this paper.

Since for finite  $U/4t$  values the Hamiltonian  $\hat{H}$  of Eq. (1) does not commute with the unitary operator  $\hat{V} = e^{-\hat{S}}$ , when expressed in terms of rotated-electron creation and annihilation operators it has an infinite number of terms and according to Eq. (3) reads,

$$\hat{H} = \hat{V} \tilde{H} \hat{V}^\dagger = \tilde{H} + [\tilde{H}, \tilde{S}] + \frac{1}{2} [[\tilde{H}, \tilde{S}], \tilde{S}] + \dots \quad (4)$$

The commutator  $[\tilde{H}, \tilde{S}]$  does not vanish except for  $U/4t \rightarrow \infty$  so that  $\hat{H} \neq \tilde{H}$  for finite values of  $U/4t$ . For  $U/4t$  very large the Hamiltonian of Eq. (4) corresponds in terms of rotated-electron creation and annihilation operators to a simple rotated-electron  $t - J$  model. In turn, the higher-order  $t/U$  terms, which become increasingly important upon decreasing  $U/4t$ , generate effective rotated-electron hopping between second, third, and more distant neighboring sites. Indeed, the products of the kinetic operators  $\tilde{T}_0$ ,  $\tilde{T}_{+1}$ , and  $\tilde{T}_{-1}$  contained in the higher-order terms of  $\tilde{S} = (t/U) [\tilde{T}_{+1} - \tilde{T}_{-1}] + \mathcal{O}(t^2/U^2)$  also appear in the Hamiltonian expression (4) in terms of rotated-electron creation and annihilation operators. In spite of the operators  $\tilde{T}_0$ ,  $\tilde{T}_{+1}$ , and  $\tilde{T}_{-1}$  generating only rotated-electron hopping between nearest-neighboring sites, their products generate effective hopping between for instance second and third neighboring sites whose real-space distance in units of the lattice spacing  $a$  is for the model on the square lattice  $\sqrt{2}a$  and  $2a$ , usually associated with transfer integrals  $t'$  and  $t''$ , respectively<sup>25</sup>.

It follows that when expressed in terms of the rotated-electron operators emerging from the specific unitary transformation considered above the simple Hubbard model (1) as given in Eq. (4) contains Hamiltonian terms associated with higher-order contributions which can be effectively described by transfer integrals  $t'$ ,  $t''$ , and of higher order. It is found in the following that for hole concentration equal to or larger than zero both the model ground state and the excited states that span the one- and two-electron subspace as defined in this paper have vanishing rotated-electron double occupancy. It follows from a Renormalization Group analysis based on the results of Refs.<sup>26,27</sup> that for intermediate and large values of  $U/4t$  obeying approximately the inequality  $U/4t \geq u_0 \approx 1.302$ , besides the original nearest-neighboring hopping processes only those involving second and third neighboring sites are relevant for the square-lattice quantum liquid described by the Hamiltonian of Eqs. (1) and (4) in the one- and two-electron subspace. The value  $U/4t = u_0 \approx 1.302$  is that where according to the results of Section VI the  $s1$  fermion spinon pairing energy reaches its maximum magnitude for small hole concentration  $0 < x \ll 1$ . Such a pairing energy is found to vanish both in the limits  $U/4t \rightarrow 0$  and  $U/4t \rightarrow \infty$ . In contrast, for the 1D model it vanishes for all  $U/4t$  values.

Hence for approximately  $U/4t \geq u_0$ , out of the infinite terms on the right-hand-side of Eq. (4) only the first few Hamiltonian terms play an active role in the physics of the Hubbard model on the square lattice in the one- and two-electron subspace. Therefore, for intermediate and large values of  $U/4t$  such a square-lattice quantum liquid can be mapped onto an effective  $t - J$  model on a square lattice with  $t$ ,  $t' = t'(U/4t)$ , and  $t'' = t''(U/4t)$  transfer integrals<sup>25</sup> for which the role of the processes associated with  $t' = t'(U/4t)$  and  $t'' = t''(U/4t)$  becomes increasingly important upon decreasing the  $U/4t$  value. For that  $U/4t$  range the latter model is equivalent to the Hubbard model on the square lattice (4) in the subspace under consideration and expressed in terms of rotated-electron creation and annihilation operators. Indeed, the  $t - J$  model constraint against double occupancy is in that subspace equivalent to expressing the Hubbard model in terms of rotated-electron creation and annihilation operators.

However, the rotated electrons are not the ultimate objects whose occupancy configurations generate the exact ground states and excited energy eigenstates. For  $U/4t > 0$  suitable occupancy configurations of the charge  $c$  fermions and spin-neutral two-spinon  $s1$  fermions simpler than those of the rotated electrons generate such states: for the square-lattice model in the one- and two-electron subspace the excited states generated by the occupancy configurations of such objects are energy eigenstates. (Actually, for 1D they refer to exact energy eigenstates for the whole Hilbert space provided that  $U/4t > 0$ .) Another advantage relative to the rotated electrons is that the processes associated with the above effective transfer integrals  $t' = t'(U/4t)$  and  $t'' = t''(U/4t)$  are implicitly contained in the  $U/4t$  dependence of the energy scales associated with the  $c$  and  $s1$  fermions spectra derived in Ref.<sup>1</sup>.

The general operator description introduced in this paper for the Hubbard model on the square lattice has two main limitations:

I) For small and intermediate values of  $U/4t$  the explicit form of the unitary operator  $\hat{V}$  associated with the rotated-electron operators as defined in this paper remains an open problem. It is known that such a unitary operator has for  $U/4t > 0$  the general form  $\hat{V} = e^{-\hat{S}}$  where the expression of  $\hat{S}$  involves only the three kinetic operators  $\hat{T}_0$ ,  $\hat{T}_{+1}$ , and  $\hat{T}_{-1}$  of Eq. (2). However, the finding of the explicit form of the  $U/4t$ -dependent functional of  $\hat{S}$  in terms of the latter three operators, valid for the whole range of finite  $U/4t$  values, is a very involved and unsolved quantum problem, beyond the reach of the present status of our scheme. Indeed, the operator description introduced in this paper has been constructed to inherently the solution of that problem being equivalent to the solution of the Hubbard model on the square lattice.

II) It turns out that the quantum problem under consideration is non-perturbative in terms of electron operators so that, in contrast to a three-dimensional (3D) isotropic Fermi liquid<sup>28</sup>, rewriting the square-lattice quantum-liquid theory emerging from the general description introduced in this paper for the model in the one- and two-electron subspace in terms of the standard formalism of many-electron physics is in general an extremely complex problem. Fortunately, such a quantum liquid dramatically simplifies when expressed in terms of the  $c$  fermion and  $s1$  fermion operators and one can rich limited but valuable information on its physics in spite of the lack of explicit information about the matrix elements between energy eigenstates. The point is that as justified below in the above subspace the  $c$  and  $s1$  fermion discrete momentum values have been constructed to inherently being good quantum numbers so that the interactions of these objects are residual<sup>1,22,32</sup>.

Concerning the Hamiltonian, the microscopic processes corresponding to the effective transfer integrals  $t' = t'(U/4t)$  and  $t'' = t''(U/4t)$  are important to characterize the type of order associated with the phases of the square-lattice quantum liquid as for instance the short-range incommensurate-spiral spin order considered in Subsection VI-B. Fortunately, for small finite hole concentrations, it is confirmed in Subsection VI-A that for simple one- and two-electron operators  $\hat{O}$  the leading operator term  $\tilde{O}$  on the right-hand side of Eq. (3) generates nearly the whole spectral weight. Hence in spite of the limitations I and II, our description provides useful information about the physics contained in the model on the square lattice. Indeed, there are several reasons why, in spite of both the explicit form of the unitary operator  $\hat{V}$  being known only for large values of  $U/4t$  and the difficulties in rewriting the theory emerging from the description introduced here in terms of the standard formalism of many-electron physics, that description is rather useful for finite values of  $U/4t$  and particularly for approximately  $U/4t \geq u_0$ . This is confirmed in Ref.<sup>1</sup> from comparison of results obtained by our description and the standard formalism of many-electron physics concerning one of the few problems where controlled and reliable approximations exist within the latter formalism for the Hubbard model on the square lattice.

For one- and two-electron operators  $\hat{O}$  the terms of the general expression (3) containing commutators involving the related operator  $\hat{S} = \tilde{S}$  are found in Section V-B to generate very little spectral weight. Hence one can reach a quite faithful representation of such operators by expressing them in terms of the  $c$  and  $s1$  fermion operators. In Subsection III-A we provide the expression of the rotated-electron creation and annihilation operators in terms of the operators of the  $c$  fermions,  $\eta$ -spinons, and spinons. The construction of the spin-neutral two-spinon composite  $s1$  bond-particle operators and corresponding  $s1$  fermion operators is a more involved problem addressed in Refs.<sup>1,18</sup>. Furthermore, in spite of the explicit form of the unitary operator  $\hat{V}$  being unknown except for  $U/4t \gg 1$ , we are able to access the

transformation laws and/or invariance of several operators and quantum objects under the corresponding electron - rotated-electron unitary transformation, what provides valuable information about the physics of the Hubbard model on the square lattice for  $U/4t > 0$ .

The physical reason why the operator terms of the general expression (3) containing commutators involving the operator  $\hat{S} = \tilde{S}$  generate very little one- and two-electron spectral weight is that the rotated electrons as defined in this paper are directly related to objects whose interactions are residual so that the leading elementary processes in terms of them generate nearly the whole spectral weight. Expression of the operator terms of Eq. (3) containing commutators involving the operator  $\hat{S} = \tilde{S}$  in terms of the operators of such objects reveals that those generate higher-order processes, whereas the elementary and leading processes are generated by the operator  $\tilde{O}$ .

In Subsection VI-B we study the  $U/4t$  dependence of the maximum magnitude  $2\Delta_0$  of the  $s1$  fermion spinon pairing energy of the Hubbard model on the square lattice for small hole concentrations  $0 < x \ll 1$ . Such an energy scale is also well defined for a larger range of finite hole concentrations yet then has a different physical meaning and plays an important role in square-lattice quantum liquid. For  $0 < x \ll 1$  it plays the role of short-range incommensurate-spiral spin order parameter. That order is absent in the 1D model for which  $2\Delta_0 = 0$ . For the square-lattice model it occurs both for  $0 < x \ll 1$  and temperatures  $0 \leq T < T_0^*$  and at half filling  $x = 0$  for  $0 < T < T_0^*$ , where  $T_0^* \approx \Delta_0/k_B$ . Our study of the  $U/4t$  dependence of the energy parameter  $2\Delta_0$  profits from combination of the description introduced here with results of the low-temperature approach of Ref.<sup>29</sup> to the half-filled model. Such an approach uses a  $CP^1$  representation and is valid below the temperature  $T_0^*$  called in that reference  $T_x$ , which marks the onset of the short-range spin order. For the specific value  $U/4t \approx 1.525$  the magnitude of  $2\Delta_0$  provided in Subsection VI-B is obtained in Ref.<sup>1</sup> from combination of the description introduced in this paper with the results of Ref.<sup>30</sup> for the spin-wave spectrum obtained by summing up an infinite set of ladder diagrams for the half-filled model in a spin-density-wave-broken symmetry ground state. Moreover, in the same subsection the spiral-incommensurate character of such a short-range spin order is studied by combining results obtained from the use of our description with the action and corresponding  $CP^1$  field theory of Refs.<sup>26,27</sup>.

A realistic program to be carried out here and in following papers includes the fulfillment of two main tasks: (i) Introducing the objects whose occupancy configurations generate the energy eigenstates that span the one- and two-electron subspace and writing the rotated-electron creation and/or annihilation operators in the expression of the one- and two-electron operators  $\hat{O}$  of Eq. (3) in terms of the operators of such objects; (ii) Finding the specific occupancy configurations of the latter objects that generate such states.

As discussed above, the expression of the operator  $\tilde{O}$  in terms of the  $c$  fermion,  $\eta$ -spinon, and spinon operators provides a rather good representation of the corresponding one- or two-electron operator  $\hat{O}$  itself. In this paper we fulfill task (i) and start solving the problems needed for the fulfillment of task (ii). The latter task is concluded in Refs.<sup>1,18</sup>, whose studies profit from the general description introduced here. Furthermore, the further construction of the square-lattice quantum liquid is fulfilled in Refs.<sup>1,22</sup>. The lack for  $U/4t > 0$  of the explicit general form of the unitary operator  $\hat{V}$  prevents the derivation of matrix elements between energy eigenstates. It is confirmed elsewhere that the information about the Hubbard model on the square lattice in the one- and two-electron subspace reached by combining different methods and approximations with the general operator description introduced in this paper clarifies important open issues of the physics contained in the model. That includes its usefulness and suitability to describe the physics of real materials<sup>1,22,32</sup>.

## B. The model global $SO(3) \times SO(3) \times U(1)$ symmetry

The studies of Ref.<sup>33</sup> reveal that for  $U/4t \rightarrow \infty$  the Hamiltonian (1) has a local  $SU(2) \times SU(2) \times U(1)$  gauge symmetry. In turn, for finite  $U/4t$  values only its interacting term is invariant under  $SU(2) \times SU(2) \times U(1)$  and therefore  $SU(2) \times SU(2) \times U(1)$  becomes a group of permissible unitary transformations. As discussed in that reference, the local  $U(1)$  canonical transformation is not the ordinary  $U(1)$  gauge subgroup of electromagnetism, but instead is a "nonlinear" transformation, i.e., a gauge transformation transforming a creation or annihilation operator into a sum of nonlinear polynomials of such operators.

Furthermore, the studies of Ref.<sup>2</sup> reveal that for on-site repulsion  $U > 0$  the above local  $SU(2) \times SU(2) \times U(1)$  gauge symmetry of the model for  $U/4t \rightarrow \infty$  can be lifted to a global  $[SU(2) \times SU(2) \times U(1)]/Z_2^2 = SO(3) \times SO(3) \times U(1)$  symmetry in the presence of the kinetic-energy hopping term of the Hamiltonian (1) with  $t > 0$  and  $U/4t > 0$ . The generator of the new found hidden global  $U(1)$  symmetry is one half the rotated-electron number of singly-occupied sites operator. As mentioned above, addition of chemical-potential and magnetic-field operator terms to the Hamiltonian (1) lowers its symmetry. However, such terms commute with it and therefore the rotated-electron occupancy configurations generate for all densities state representations of its global symmetry.

Since the expression of the operator  $\hat{S}$  involves only the three kinetic operators  $\hat{T}_0$ ,  $\hat{T}_{+1}$ , and  $\hat{T}_{-1}$  given in Eq. (2),

the electron - rotated-electron unitary operator  $\hat{V} = \tilde{V}$  preserves the occurrence of nearest hopping only for rotated electrons alike for electrons and commutes with the momentum operator  $\hat{\vec{P}}$  and, therefore, according to Eq. (3) the latter operator is such that  $\hat{\vec{P}} = \tilde{\vec{P}}$  and thus has the same expression in terms of electron and rotated-electron creation and annihilation operators,

$$\hat{\vec{P}} = \sum_{\sigma=\uparrow,\downarrow} \sum_{\vec{k}} \vec{k} c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} = \sum_{\sigma=\uparrow,\downarrow} \sum_{\vec{k}} \vec{k} \tilde{c}_{\vec{k},\sigma}^\dagger \tilde{c}_{\vec{k},\sigma}. \quad (5)$$

In addition, according to the studies of Ref.<sup>2</sup> the unitary operator  $\hat{V}$  commutes with the three generators of the spin  $SU(2)$  symmetry and three generators of the  $\eta$ -spin  $SU(2)$  symmetry. Hence, such generators also have the same expression in terms of electron and rotated-electron creation and annihilation operators and read,

$$\begin{aligned} \hat{S}_\eta^z &= -\frac{1}{2}[N_a^D - \hat{N}]; \quad \hat{S}_s^z = -\frac{1}{2}[\hat{N}_\uparrow - \hat{N}_\downarrow], \\ \hat{S}_\eta^\dagger &= \sum_{j=1}^{N_a^D} e^{i\vec{\pi} \cdot \vec{r}_j} c_{\vec{r}_j,\downarrow}^\dagger c_{\vec{r}_j,\uparrow} = \sum_{j=1}^{N_a^D} e^{i\vec{\pi} \cdot \vec{r}_j} \tilde{c}_{\vec{r}_j,\downarrow}^\dagger \tilde{c}_{\vec{r}_j,\uparrow}; \quad \hat{S}_\eta = \sum_{j=1}^{N_a^D} e^{-i\vec{\pi} \cdot \vec{r}_j} c_{\vec{r}_j,\uparrow} c_{\vec{r}_j,\downarrow} = \sum_{j=1}^{N_a^D} e^{-i\vec{\pi} \cdot \vec{r}_j} \tilde{c}_{\vec{r}_j,\uparrow} \tilde{c}_{\vec{r}_j,\downarrow}, \\ \hat{S}_s^\dagger &= \sum_{j=1}^{N_a^D} c_{\vec{r}_j,\downarrow}^\dagger c_{\vec{r}_j,\uparrow} = \sum_{j=1}^{N_a^D} \tilde{c}_{\vec{r}_j,\downarrow}^\dagger \tilde{c}_{\vec{r}_j,\uparrow}; \quad \hat{S}_s = \sum_{j=1}^{N_a^D} c_{\vec{r}_j,\uparrow} c_{\vec{r}_j,\downarrow} = \sum_{j=1}^{N_a^D} \tilde{c}_{\vec{r}_j,\uparrow}^\dagger \tilde{c}_{j,\downarrow}, \end{aligned} \quad (6)$$

where for the model on the square (and 1D) lattice the vector  $\vec{\pi}$  has Cartesian components  $\vec{\pi} = [\pi, \pi]$  (and component  $\pi$ ).

In turn, alike the Hamiltonian of Eq. (1), the generator  $\tilde{S}_c$  of the charge independent  $U(1)$  symmetry does not commute with the unitary operator  $\hat{V}$ . On the contrary of the Hamiltonian, that operator has a complicated expression in terms of electron creation and annihilation operators and a simple expression in terms of rotated-electron creation and annihilation operators<sup>2</sup>, which reads,

$$\tilde{S}_c = \frac{1}{2} \sum_{j=1}^{N_a^D} \sum_{\sigma=\uparrow,\downarrow} \tilde{n}_{\vec{r}_j,\sigma} (1 - \tilde{n}_{\vec{r}_j,-\sigma}). \quad (7)$$

It follows that  $\tilde{S}_c = \hat{V}^\dagger \hat{S}_c \hat{V}$  where  $\hat{S}_c = \frac{1}{2}\hat{Q}$  and the operator  $\hat{Q}$  is given in Eq. (1). The six operators provided in Eq. (6) plus that given in Eq. (7) are the seven generators of the group  $[SO(4) \times U(1)]/Z_2 = SO(3) \times SO(3) \times U(1)$  associated with the global symmetry of the Hamiltonian (1).

That for  $U/4t > 0$  the eigenvalue  $S_c$  of the generator (7) is a good quantum number implies that the rotated-electron doubly occupancy  $D_c = [N/2 - S_c]$  is also a good quantum number. Alike for the more general case considered in Ref.<sup>2</sup>, following the unitary character of the operator  $\hat{V} = \tilde{V}$  associated with the rotated electrons as constructed in this paper one can either consider that  $\hat{V} \hat{H} \hat{V}^\dagger = \tilde{H} + [\tilde{H}, \tilde{S}] + \dots$  is the Hubbard model written in terms of rotated-electron operators or another Hamiltonian with an involved expression and whose operators  $\tilde{c}_{\vec{r}_j,\sigma}^\dagger$  and  $\tilde{c}_{\vec{r}_j,\sigma}$  correspond to electrons. The studies of Ref.<sup>2</sup> refer to any unitary operator  $\hat{V}$  associated with the general type of unitary transformations considered in Ref.<sup>11</sup>. In turn, the operator  $\hat{V}$  used here corresponds to a suitable set of  $4^{N_a^D}$   $U/4t \rightarrow \infty$  energy eigenstates  $\{|\Psi_\infty\rangle\}$  such that for  $U/4t > 0$  the  $V$  tower states  $|\Psi_{U/4t}\rangle = \hat{V}^\dagger |\Psi_\infty\rangle$  are energy and momentum eigenstates. In the more general case considered in that reference the  $4^{N_a^D}$  states  $\hat{V}^\dagger |\Psi_\infty\rangle$  are eigenstates of the generator of the charge  $U(1)$  symmetry and of the  $\eta$ -spin and spin square operators of the  $SU(2)$  symmetries so that the values of  $S_c$ ,  $S_\eta$ , and  $S_s$  are well defined yet such states are not in general energy and momentum eigenstates.

Following the procedures of Ref.<sup>11</sup>, the Hamiltonian  $\hat{V} \hat{H} \hat{V}^\dagger = \tilde{H} + [\tilde{H}, \tilde{S}] + \dots$  is built up by use of the conservation of singly occupancy  $2S_c = \langle \hat{Q} \rangle$  by eliminating terms in the  $t > 0$  Hubbard Hamiltonian so that  $S_c$  is an eigenvalue of the operator (7). According to the studies of that reference this can be done to all orders of  $4t/U$  provided that  $U/4t \neq 0$ . The original lattice remains invariant under the electron - rotated-electron unitary transformation and the energy eigenstate description introduced in this paper has been constructed to inherently each site of that lattice being unoccupied, doubly occupied, singly occupied by a spin-up rotated electron, or singly occupied by a spin-down rotated electron.

### III. THREE ELEMENTARY QUANTUM OBJECTS AND CORRESPONDING $c$ , $\eta$ -SPIN, AND SPIN EFFECTIVE LATTICES

#### A. Elementary quantum objects and their operators

The rotated electrons are not the ultimate objects whose occupancy configurations that generate the energy eigenstates of the model (1) in the one- and two-electron subspace have simplest expressions. There emerge from the electron - rotated-electron unitary transformation considered here three basic objects: the spin-less and  $\eta$ -spin-less  $c$  fermions, the spin-1/2 spinons, and the  $\eta$ -spin-1/2  $\eta$ -spinons. Such objects are a generalization for  $U/4t > 0$  of those introduced in Ref.<sup>12</sup> for  $U/4t \gg 1$ , as discussed below. In Appendix B it is confirmed that for the 1D Hubbard model and all  $U/4t$  values suitable occupancy configurations of such objects generate a complete set of energy eigenstates, which span the whole Hilbert space. In this paper and in Ref.<sup>1</sup> evidence is provided that suitable  $c$  and  $s1$  fermion momentum occupancy configurations generate the exact ground states and the excited energy eigenstates that span the one- and two-electron subspace defined below in Section V.

Here we profit from the result of Appendix A that full information about the quantum problem can be achieved by defining it in the LWS-subspace. Within the corresponding LWS representation the  $c$  fermion creation operator can be expressed in terms of the rotated-electron operators and electron operators as follows,

$$\begin{aligned} f_{\vec{r}_j,c}^\dagger &= \tilde{c}_{\vec{r}_j,\uparrow}^\dagger (1 - \tilde{n}_{\vec{r}_j,\downarrow}) + e^{i\vec{\pi} \cdot \vec{r}_j} \tilde{c}_{\vec{r}_j,\uparrow} \tilde{n}_{\vec{r}_j,\downarrow}; & f_{\vec{q}_j,c}^\dagger &= \frac{1}{\sqrt{N_a^D}} \sum_{j'=1}^{N_a^D} e^{+i\vec{q}_j \cdot \vec{r}_{j'}} f_{\vec{r}_{j'},c}^\dagger, \\ \tilde{n}_{\vec{r}_j,\sigma} &= \tilde{c}_{\vec{r}_j,\sigma}^\dagger \tilde{c}_{\vec{r}_j,\sigma}; & \tilde{c}_{\vec{r}_j,\sigma}^\dagger &= \hat{V}^\dagger c_{\vec{r}_j,\sigma}^\dagger \hat{V}; & \tilde{c}_{\vec{r}_j,\sigma} &= \hat{V}^\dagger c_{\vec{r}_j,\sigma} \hat{V}, \end{aligned} \quad (8)$$

where we have introduced the corresponding  $c$  fermion momentum-dependent operators as well,  $e^{i\vec{\pi} \cdot \vec{r}_j}$  is  $\pm 1$  depending on which sublattice site  $\vec{r}_j$  is on, and  $\hat{V}^\dagger$  is the uniquely defined electron - rotated-electron unitary operator introduced in this paper. (For the 1D lattice that phase factor can be written as  $(-1)^j$ .) The expression in terms of electron operators involves the electron - rotated-electron unitary operator  $\hat{V}$  as defined in this paper. The  $c$  momentum band is studied in Ref.<sup>1</sup> and has the same shape and momentum area as the electronic first-Brillouin zone.

The three spinon local operators  $s_{\vec{r}_j}^l$  and three  $\eta$ -spinon local operators  $p_{\vec{r}_j}^l$  such that  $l = \pm, z$  are given by,

$$s_{\vec{r}_j}^l = n_{\vec{r}_j,c} q_{\vec{r}_j}^l; \quad p_{\vec{r}_j}^l = (1 - n_{\vec{r}_j,c}) q_{\vec{r}_j}^l, \quad l = \pm, z. \quad (9)$$

Here  $q_{\vec{r}_j}^\pm = q_{\vec{r}_j}^x \pm i q_{\vec{r}_j}^y$  are the rotated quasi-spin operators whose Cartesian coordinates  $x, y, z$  are often denoted in this paper by  $x_1, x_2, x_3$ , respectively, and,

$$n_{\vec{r}_j,c} = f_{\vec{r}_j,c}^\dagger f_{\vec{r}_j,c}, \quad (10)$$

is the  $c$  fermion local density operator.

In terms of rotated-electron creation and annihilation operators the rotated quasi-spin operators read,

$$q_{\vec{r}_j}^+ = (\tilde{c}_{\vec{r}_j,\uparrow}^\dagger - e^{i\vec{\pi} \cdot \vec{r}_j} \tilde{c}_{\vec{r}_j,\uparrow}) \tilde{c}_{\vec{r}_j,\downarrow}; \quad q_{\vec{r}_j}^- = (q_{\vec{r}_j}^+)^{\dagger}; \quad q_{\vec{r}_j}^z = \frac{1}{2} - \tilde{n}_{\vec{r}_j,\downarrow}. \quad (11)$$

Since the electron - rotated-electron transformation generated by the operator  $\hat{V}$  is unitary, the operators  $\tilde{c}_{\vec{r}_j,\sigma}^\dagger$  and  $\tilde{c}_{\vec{r}_j,\sigma}$  have the same anticommutation relations as  $c_{\vec{r}_j,\sigma}^\dagger$  and  $c_{\vec{r}_j,\sigma}$ , respectively. Straightforward manipulations based on Eqs. (8)-(11) then lead to the following algebra for the  $c$  fermion operators,

$$\{f_{\vec{r}_j,c}^\dagger, f_{\vec{r}_{j'},c}\} = \delta_{j,j'}; \quad \{f_{\vec{r}_j,c}^\dagger, f_{\vec{r}_{j'},c}^\dagger\} = \{f_{\vec{r}_j,c}, f_{\vec{r}_{j'},c}\} = 0, \quad (12)$$

$c$  fermion operators and rotated quasi-spin operators,

$$[f_{\vec{r}_j,c}^\dagger, q_{\vec{r}_{j'}}^l] = [f_{\vec{r}_j,c}, q_{\vec{r}_{j'}}^l] = 0, \quad (13)$$

and rotated quasi-spin operators,

$$[q_{\vec{r}_j}^p, q_{\vec{r}_{j'}}^{p'}] = i \delta_{j,j'} \sum_{p''} \epsilon_{pp'p''} q_{\vec{r}_j}^{p''}; \quad p = x, y, z, \quad (14)$$



$$\{q_{\vec{r}_j}^+, q_{\vec{r}_j}^-\} = 1, \quad \{q_{\vec{r}_j}^\pm, q_{\vec{r}_j'}^\pm\} = 0, \quad (15)$$

$$[q_{\vec{r}_j}^+, q_{\vec{r}_j'}^-] = [q_{\vec{r}_j}^\pm, q_{\vec{r}_j'}^\pm] = 0. \quad (16)$$

Hence the operators  $q_{\vec{r}_j}^\pm$  anticommute on the same site and commute on different sites.

The relations provided in Eqs. (12)-(16) confirm that the  $c$  fermions associated with the global  $U(1)$  symmetry are  $\eta$ -spinless and spinless fermionic objects and the spinons and  $\eta$ -spinons are spin-1/2 and  $\eta$ -spin-1/2 objects whose local operators obey the usual corresponding spin and  $\eta$ -spin  $SU(2)$  algebras, respectively.

We can now fulfill task (i) suggested in Subsection II-A: Writing the rotated-electron creation and/or annihilation operators in the expression of any one- or two-electron operator  $\hat{O}$  of Eq. (3) in terms of the operators of the objects whose simple occupancy configurations generate the energy eigenstates that span the one- and two-electron subspace of the model on the square lattice and the whole Hilbert space of the 1D model. For the LWS-subspace considered here this is simply achieved by inverting the relations given in Eqs. (8) and (11) with the result,

$$\hat{c}_{\vec{r}_j, \uparrow}^\dagger = f_{\vec{r}_j, c}^\dagger \left( \frac{1}{2} + q_{\vec{r}_j}^z \right) + e^{i\vec{\pi} \cdot \vec{r}_j} f_{\vec{r}_j, c} \left( \frac{1}{2} - q_{\vec{r}_j}^z \right); \quad \hat{c}_{\vec{r}_j, \downarrow}^\dagger = q_{\vec{r}_j}^- (f_{\vec{r}_j, c}^\dagger - e^{i\vec{\pi} \cdot \vec{r}_j} f_{\vec{r}_j, c}). \quad (17)$$

For  $U/4t \rightarrow \infty$  the rotated electrons become electrons and Eqs. (8)-(17) are equivalent to Eqs. (1)-(3) of Ref.<sup>12</sup> with the rotated-electron operators replaced by the corresponding electron operators and the  $c$  fermion creation operator  $f_{\vec{r}_j, c}^\dagger$  replaced by the quasicharge annihilation operator  $\hat{c}_r$ . Therefore, in that limit the  $c$  fermions are the "holes" of the quasicharge particles of that reference and the spinons and  $\eta$ -spinons are associated with the local spin and pseudospin operators, respectively.

Since the transformation considered in Ref.<sup>12</sup> does not introduce Hilbert-space constraints, suitable occupancy configurations of the objects associated with the local quasicharge, spin, and pseudospin operators generate a complete set of states. However, only in the  $U/4t \rightarrow \infty$  limit simple occupancy configurations of the corresponding quasicharge, spin, and pseudospin objects generate the energy eigenstates that span the one- and two-electron subspace. In turn, for the model on the square lattice the same occupancy configurations of the above corresponding finite- $U/4t$  objects generate the energy eigenstates belonging to the same  $V$  tower.

Our next main goal is the fulfillment of the task (ii) also suggested in Subsection II-A: Finding the suitable occupancy configurations of the  $c$  fermions, spinons, and  $\eta$ -spinons that generate energy eigenstates of the one- and two-electron subspace. The study of the relationship of the transformation laws of such objects under the electron - rotated-electron unitary transformation to the state representations of the group  $SO(3) \times SO(3) \times U(1)$  associated with the model global symmetry provides valuable and useful yet partial information about that complex problem. Here we start a preliminary analysis of the degrees of freedom of the rotated-electron occupancy configurations that generate a complete set of  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ , and  $S_c$  eigenstates and introduce the theory vacua. Such  $4^{N_a^D}$  states correspond to representations of the model global  $SO(3) \times SO(3) \times U(1)$  symmetry. As discussed in Section IV, they are momentum eigenstates of the square-lattice model in the whole Hilbert space. For the 1D Hubbard model the states of such a complete set are shown in Appendix B to be both momentum and energy eigenstates.

### B. Interplay of the global symmetry with the transformation laws under the operator $\hat{V}$ : three basic effective lattices and the theory vacua

The rotated-electron occupancy configurations associated with the state representations of the global  $SO(3) \times SO(3) \times U(1) = [SU(2) \times SU(2) \times U(1)]/Z_2^2$  symmetry are well defined for  $U/4t > 0$ . It is found in Subsection IV-D that the  $\eta$ -spin and spin state representations correspond to independent rotated-electron occupancy configurations of  $[N_a^D - 2S_c]$  sites and  $2S_c$  sites, respectively, whereas the  $U(1)$  symmetry refers to the relative positions of the sites involved in each of these two types of configurations. In the present  $N_a \gg 1$  limit it is useful to introduce the numbers  $N_{a_\eta}$  and  $N_{a_s}$  such that  $N_{a_\eta}^D = [N_a^D - 2S_c]$  and  $N_{a_s}^D = 2S_c$ ,

$$N_{a_\eta} = (N_a^D - 2S_c)^{1/D}; \quad N_{a_s} = (2S_c)^{1/D}; \quad N_a^D = N_{a_\eta}^D + N_{a_s}^D. \quad (18)$$

Here  $N_{a_\eta}^D$  and  $N_{a_s}^D$  are integer numbers that below are identified with the number of sites of a  $\eta$ -spin and spin effective lattice, respectively. For the  $D = 2$  square lattice the number  $N_a^D$  is chosen so that the number  $N_a$  of sites in a row or column is an integer. However, the designations  $N_{a_\eta}^D$  and  $N_{a_s}^D$  do not imply that the corresponding numbers  $N_{a_\eta}$  and  $N_{a_s}$  are integers. In general they are not integers but for finite values of  $x$  and  $(1 - x)$  the closest integer numbers to

$N_{a_\eta}$  and  $N_{a_s}$  give the mean value of the number of sites in a row or column of the  $\eta$ -spin and spin effective lattices, respectively.

The degrees of freedom of the rotated-electron occupancy configurations of each of the  $N_{a_\eta}^D = [N_a^D - 2S_c]$  and  $N_{a_s}^D = 2S_c$  sites of the original lattice that generate the  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ , and  $S_c$  eigenstates studied in Section IV, which correspond to state representations of the model global  $SO(3) \times SO(3) \times U(1)$  symmetry, naturally separate as follows:

i) The occupancy configurations of the  $c$  fermions associated with the operators  $f_{\vec{r}_j,c}^\dagger$  of Eq. (8) where  $j = 1, \dots, N_{a_\eta}^D$  correspond to the state representations of the global  $U(1)$  symmetry found in Ref.<sup>2</sup>. Such  $c$  fermions live on the  $c$  effective lattice, which is identical to the original lattice. Its occupancies are related to those of the rotated electrons, the number of  $c$  fermion occupied and unoccupied sites being given by  $N_c = N_{a_s}^D = 2S_c$  and  $N_c^h = N_{a_\eta}^D = [N_a^D - 2S_c]$ , respectively. Indeed, the  $c$  fermions occupy the sites singly occupied by the rotated electrons whereas the rotated-electron doubly-occupied and unoccupied sites are those unoccupied by the  $c$  fermions. Hence the  $c$  fermion occupancy configurations describe the relative positions in the original lattice of the  $N_{a_\eta}^D = [N_a^D - 2S_c]$  sites of the  $\eta$ -spin effective lattice and  $N_{a_s}^D = 2S_c$  sites of the spin effective lattice.

ii) In turn, the remaining degrees of freedom of rotated-electron occupancies of the  $N_{a_\eta}^D = [N_a^D - 2S_c]$  and  $N_{a_s}^D = 2S_c$  original lattice sites correspond to the occupancy configurations associated with the  $\eta$ -spin  $SU(2)$  symmetry and spin  $SU(2)$  symmetry representations, respectively. The occupancy configurations of the  $N_{a_\eta}^D = [N_a^D - 2S_c]$  sites of the  $\eta$ -spin effective lattice and  $N_{a_s}^D = 2S_c$  sites of the spin effective lattice are independent. They refer to the operators  $p_{\vec{r}_j}^l$  of Eq. (9), which act only onto the  $N_{a_\eta}^D = [N_a^D - 2S_c]$  sites of the  $\eta$ -spin effective lattice, and to the operators  $s_{\vec{r}_j}^l$  given in the same equation, which act onto the  $N_{a_s}^D = 2S_c$  sites of the spin effective lattice, respectively. This is assured by the operators  $(1 - n_{\vec{r}_j,c})$  and  $n_{\vec{r}_j,c}$  in their expressions provided in that equation, which play the role of projectors onto the  $\eta$ -spin and spin effective lattice, respectively.

It follows that for  $U/4t > 0$  the degrees of freedom of each rotated-electron singly occupied site separate into a spin-less  $c$  fermion carrying the electronic charge and a spin-down or spin-up spinon. Furthermore, the degrees of freedom of each rotated-electron doubly-occupied or unoccupied site separate into a  $\eta$ -spin-less  $c$  fermion hole and a  $\eta$ -spin-down or  $\eta$ -spin-up  $\eta$ -spinon, respectively. The  $\eta$ -spin-down or  $\eta$ -spin-up  $\eta$ -spinon refers to the  $\eta$ -spin degrees of freedom of a rotated-electron doubly-occupied or unoccupied site, respectively, of the original lattice. Above and in the remaining of this paper we often call  $c$  fermion hole an unoccupied site of the  $c$  effective lattice.

A key point of our description is that for  $U/4t > 0$  its quantum objects correspond to rotated-electron configurations whose spin-down and spin-up singly occupancy, doubly occupancy, and no occupancy refer to good quantum numbers. This is in contrast to descriptions in terms of electronic configurations, whose singly occupancy refers to a good quantum number for  $U/4t \gg 1$  only<sup>6,21,34,35</sup>.

The transformation laws of the  $\eta$ -spinons (and spinons) under the electron - rotated-electron unitary transformation associated with the operator  $\hat{V}$  play a major role in the description of the  $\eta$ -spin (and spin) state representations in terms of occupancy configurations of the  $N_{a_\eta}^D = [N_a^D - 2S_c]$  sites of the  $\eta$ -spin effective lattice (and  $N_{a_s}^D = 2S_c$  sites of the spin effective lattice). Importantly, a well-defined number of  $\eta$ -spinons (and spinons) remain invariant under the unitary transformation generated by  $\hat{V}$ . Those are called independent  $\pm 1/2$   $\eta$ -spinons (and independent  $\pm 1/2$  spinons) and as further discussed below play the role of unoccupied sites of the  $\eta$ -spin (and spin) effective lattice. The values of the numbers  $L_{\eta, \pm 1/2}$  of independent  $\pm 1/2$   $\eta$ -spinons and  $L_{s, \pm 1/2}$  of independent  $\pm 1/2$  spinons are fully controlled by those of the  $\eta$ -spin  $S_\eta$  and  $\eta$ -spin projection  $S_\eta^z = -x N_a^D$  and spin  $S_s$  and spin projection  $S_s^z = -m N_a^D$ , respectively, and are given by,

$$L_\alpha = [L_{\alpha, -1/2} + L_{\alpha, +1/2}] = 2S_\alpha; \quad L_{\alpha, \pm 1/2} = [S_\alpha \mp S_\alpha^z]; \quad \alpha = \eta, s. \quad (19)$$

The invariance of such independent  $\eta$ -spinons (and spinons) stems from the off diagonal generators of the  $\eta$ -spin (and spin) algebra, which flip their  $\eta$ -spin (and spin), commuting with the unitary operator  $\hat{V}$  and hence having for  $U/4t > 0$  the same expressions in terms of electron and rotated-electron operators, as given in Eq. (6).

It follows that the number of sites of the  $\eta$ -spin ( $\alpha = \eta$ ) and spin ( $\alpha = s$ ) effective lattice can be written as,

$$N_{a_\alpha}^D = [2S_\alpha + 2C_\alpha]; \quad \alpha = \eta, s. \quad (20)$$

The occupancy configurations of  $2S_\alpha$  sites out of  $N_{a_\alpha}^D$  have for  $U/4t > 0$  the same form in terms of electrons and rotated electrons. However, that refers to the  $\eta$ -spin or spin effective lattices and hence only to the  $\eta$ -spin ( $\alpha = \eta$ ) or spin ( $\alpha = s$ ) degrees of freedom, respectively, of the rotated-electron occupancies of the original lattice. Indeed, for finite values of  $U/4t$  and spin density  $m < (1 - x)$  the  $c$  fermion occupancy configurations are not invariant under the electron - rotated-electron unitary transformation.

Nevertheless, the two sets of  $2S_\eta$  and  $2C_\eta$  (and  $2S_s$  and  $2C_s$ ) sites of the  $\eta$ -spin (and spin) effective lattice correspond to two well-defined sets of  $2S_\eta$  and  $2C_\eta$  (and  $2S_s$  and  $2C_s$ ) sites of the original lattice. Out of the set of  $2S_\eta = [L_{\eta,-1/2} + L_{\eta,+1/2}]$  (and  $2S_s = [L_{s,-1/2} + L_{s,+1/2}]$ ) sites of the original lattice,  $L_{\eta,-1/2}$  are doubly occupied and  $L_{\eta,+1/2}$  unoccupied both by electrons and rotated electrons (and  $L_{s,-1/2}$  and  $L_{s,+1/2}$  are singly occupied both by spin-down and spin-up, respectively, electrons and rotated electrons.) Out of the  $2C_\eta$  (and  $2C_s$ ) sites of the original lattice left over, the corresponding  $C_\eta$  (and  $C_s$ ) sites are unoccupied by rotated electrons (and singly occupied by spin-up rotated electrons) and the remaining  $C_\eta$  (and  $C_s$ ) sites are doubly occupied by rotated electrons (and singly occupied by spin-down rotated electrons). In turn, in terms of electrons these  $[2C_\eta + 2C_s]$  sites of the original lattice have for finite  $U/4t$  values very involved occupancies such that singly and doubly occupancy are not good quantum numbers and thus are not conserved.

The site numbers  $C_\eta \geq 0$  and  $C_s \geq 0$  are good quantum numbers given by,

$$C_\eta = [N_{a_\eta}^D/2 - S_\eta] = [N_a^D/2 - S_c - S_\eta]; \quad C_s = [N_{a_s}^D/2 - S_s] = [S_c - S_s]. \quad (21)$$

Hence their values are fully determined by those of the eigenvalue  $S_c$  of the global  $U(1)$  symmetry generator and  $\eta$ -spin  $S_\eta$  or spin  $S_s$ , respectively, so that  $C_\eta$  and  $C_s$  are not independent quantum numbers.

The physics behind the  $U(1)$  symmetry found in Ref.<sup>2</sup> includes that brought about by the rotated-electron occupancy configurations of the  $[2C_\eta + 2C_s]$  sites of Eq. (21). The use of the corresponding model global  $SO(3) \times SO(3) \times U(1)$  symmetry confirms that the integer numbers  $2C_\alpha \geq 0$  are always even and that application onto  $S_\alpha = 0$  states of the off-diagonal generators of the  $\eta$  spin ( $\alpha = \eta$ ) or spin ( $\alpha = s$ ) algebra provided in Eq. (6) gives zero. For such states  $N_{a_\alpha}^D = 2C_\alpha$ .

On the other hand, application of these generators onto  $2S_\alpha > 0$  states flips the  $\eta$ -spin ( $\alpha = \eta$ ) or spin ( $\alpha = s$ ) of an independent  $\eta$ -spinon ( $\alpha = \eta$ ) or independent spinon ( $\alpha = s$ ) but leaves invariant the rotated-electron occupancy configurations of the above considered  $2C_\alpha$  sites. It follows that such  $2C_\eta$  (and  $2C_s$ ) sites refer to  $\eta$ -spin-singlet (and spin-singlet) configurations involving  $C_\eta$  (and  $C_s$ )  $-1/2$   $\eta$ -spinons (and  $-1/2$  spinons) and an equal number of  $+1/2$   $\eta$ -spinons (and  $+1/2$  spinons).

One then concludes that concerning the rotated-electron occupancies of the original lattice, besides the  $[2S_\eta + 2S_s]$  sites whose occupancies are the same in terms of electrons and rotated electrons, there are  $C_\eta \geq 0$  sites doubly occupied by rotated electrons,  $C_\eta \geq 0$  sites unoccupied by rotated electrons,  $C_s \geq 0$  sites singly occupied by spin-down rotated electrons, and  $C_s \geq 0$  sites singly occupied by spin-up rotated electrons.

Let  $M_\alpha = M_{\alpha,-1/2} + M_{\alpha,+1/2}$  denote the total number of  $\eta$ -spinons ( $\alpha = \eta$ ) and spinons ( $\alpha = s$ ). It is given by  $M_\alpha = N_{a_\alpha}^D$  and hence  $M_\eta = N_{a_\eta}^D = [N_a^D - 2S_c]$  and  $M_s = N_{a_s}^D = 2S_c$ . Out of the  $M_\eta = N_{a_\eta}^D = [N_a^D - 2S_c]$   $\eta$ -spinons (and  $M_s = N_{a_s}^D = 2S_c$  spinons),  $L_\eta = 2S_\eta$  (and  $L_s = 2S_s$ ) are invariant under the unitary operator  $\hat{V}$  and  $2C_\eta = [M_\eta - 2S_\eta]$  (and  $2C_s = [M_s - 2S_s]$ ) are not invariant under that unitary operator. Also the  $c$  fermions are not invariant under  $\hat{V}$ . Indeed, the generators of the occupancy configurations of the latter objects are for finite values of  $U/4t$  and  $m < (1 - x)$  different when expressed in terms of rotated-electron and electron operators, respectively. The number of  $\eta$ -spinons ( $\alpha = \eta$ ) and spinons ( $\alpha = s$ ) can then be written as,

$$M_{\alpha,\pm 1/2} = [L_{\alpha,\pm 1/2} + C_\alpha]; \quad M_\alpha = N_{a_\alpha}^D = [2S_\alpha + 2C_\alpha]; \quad \alpha = \eta, s. \quad (22)$$

The  $\eta$ -spinon and spinon operator algebra refers to well-defined subspaces spanned by states whose number of each of these basic objects is constant and given by  $M_\eta = N_{a_\eta}^D = [N_a^D - 2S_c]$  and  $M_s = N_{a_s}^D = 2S_c$ , respectively. Hence in such subspaces the number  $2S_c$  of rotated-electron singly occupied sites and the numbers  $N_{a_\eta}^D$  and  $N_{a_s}^D$  of sites of the  $\eta$ -spin and spin effective lattices, respectively, are constant. For hole concentrations  $0 \leq x < 1$  and maximum spin density  $m = (1 - x)$  reached at a critical magnetic field  $H_c$  parallel to the square-lattice plane for  $D = 2$  and pointing along the chain for  $D = 1$  the  $c$  fermion operators are invariant under the electron - rotated-electron unitary transformation and there is a fully polarized vacuum  $|0_{\eta s}\rangle$ , which remains invariant under such a transformation. It reads,

$$|0_{\eta s}\rangle = |0_\eta; N_{a_\eta}^D\rangle \times |0_s; N_{a_s}^D\rangle \times |GS_c; 2S_c\rangle, \quad (23)$$

where the  $\eta$ -spin  $SU(2)$  vacuum  $|0_\eta; N_{a_\eta}^D\rangle$  associated with  $N_{a_\eta}^D$  independent  $+1/2$   $\eta$ -spinons, the spin  $SU(2)$  vacuum  $|0_s; N_{a_s}^D\rangle$  with  $N_{a_s}^D$  independent  $+1/2$  spinons, and the  $c$   $U(1)$  vacuum  $|GS_c; 2S_c\rangle$  with  $N_c = 2S_c$   $c$  fermions remain invariant under the electron - rotated-electron unitary transformation. The explicit expression of the state  $|GS_c; 2S_c\rangle$  used below in Subsection IV-E is  $\prod_{\vec{q}} f_{\vec{q},c}^\dagger |GS_c; 0\rangle$  where the vacuum  $|GS_c; 0\rangle$  corresponds to the electron and rotated-electron vacuum of form (23) referring to  $N_{a_\eta}^D = N_a^D$  and  $N_{a_s}^D = 2S_c = 0$ . Only for a  $m = (1 - x)$  fully polarized state are the state  $|GS_c; 2S_c\rangle$  and the corresponding  $N_c = 2S_c$  fermions invariant under the electron - rotated-electron unitary transformation for  $U/4t > 0$ . For the vacuum  $|0_\eta; N_{a_\eta}^D\rangle$  (and  $|0_s; N_{a_s}^D\rangle$ ) the  $M_\eta = N_{a_\eta}^D$  independent  $+1/2$

$\eta$ -spinons refer to  $N_{a_\eta}^D$  sites of the original lattice unoccupied by rotated electrons (and the  $M_s = N_{a_s}^D$  independent  $+1/2$  spinons to the spins of  $N_{a_s}^D$  spin-up rotated electrons that singly occupy sites of such a lattice). At maximum spin density  $m = (1 - x)$  the  $c$  fermions are the non-interacting spinless fermions that describe the charge degrees of freedom of the electrons of the fully polarized ground state. At that spin density there are no electron doubly occupied sites and the quantum problem is non-interacting for  $U/4t > 0$ .

The studies of Ref.<sup>1</sup> reveal that the  $x = 0$  and  $m = 0$  absolute ground state such that  $N_{a_\eta}^D = 0$ ,  $N_{a_s}^D = N_a^D = 2N_{s1}$ , and  $2S_c = N_a^D$  where  $N_{s1}$  is the number of  $s1$  fermions considered below is also invariant under the electron - rotated-electron transformation. Such an invariance is related to the Mott-Hubbard insulator physics. This is consistent with the  $S_c = N_a^D/2$  vacuum referring to a spin-up fully polarized state, whose numbers are also  $N_{a_\eta}^D = 0$ ,  $N_{a_s}^D = N_a^D$ , and  $2S_c = N_a^D$  and correspond to a particular case of the general state (23), being invariant under that transformation.

Following the result of Appendix A that full information about the quantum problem described by the Hamiltonian (1) can be achieved by defining it in the LWS-subspace spanned by states such that  $L_{\alpha, -1/2} = 0$  and  $L_{\alpha, +1/2} = 2S_\alpha$  for  $\alpha = \eta, s$ , in the ensuing section we confirm that within the description introduced in this paper, out of the  $N_{a_\alpha}^D = [2S_\alpha + 2C_\alpha]$  sites of the  $\eta$ -spin ( $\alpha = \eta$ ) and spin ( $\alpha = s$ ) effective lattice, the  $2S_\alpha$  lattices whose occupancies are invariant under  $\hat{V}$  play the role of unoccupied sites, whereas the remaining  $2C_\alpha$  sites play the role of occupied sites. This is a natural consequence of the  $\eta$ -spin  $SU(2)$  vacuum  $|0_\eta; N_{a_\eta}^D\rangle$  (and spin  $SU(2)$  vacuum  $|0_s; N_{a_s}^D\rangle$ ) being for all  $U/4t$  and  $m$  values invariant under the electron - rotated-electron unitary transformation and such that  $N_{a_\eta}^D = 2S_\eta$  so that  $2C_\eta = 0$  (and  $N_{a_s}^D = 2S_s$  so that  $2C_s = 0$ ).

#### IV. COMPOSITE $\alpha\nu$ FERMIONS, $\alpha\nu$ BOND PARTICLES, AND CORRESPONDING $\alpha\nu$ EFFECTIVE LATTICES

In this section we consider a uniquely chosen complete set of  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates that within the present description for the Hubbard model on the 1D or square lattices is generated by  $c$  fermion,  $\eta$ -spinon, and spinon occupancy configurations. As discussed in Appendix B, for the 1D Hubbard model with  $U/4t > 0$  such states are a complete set of energy eigenstates. For the model on the square lattice such states are in some particular cases energy eigenstates, including ground states and the states that span the one- and two-electron subspace as defined in Section V. Here we access partial yet valuable information about the  $\eta$ -spinon and spinon occupancy configurations that generate the  $\eta$ -spin and spin degrees of freedom of such  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates from the suitable use of the transformations laws of the above objects under the electron - rotated-electron unitary transformation.

Specifically, within the general description introduced in this paper both for the Hubbard model on the square and 1D lattice, the complete set of  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates can in the  $N_a^D \rightarrow \infty$  limit be generated by occupancy configurations of  $c$  fermions, several branches of composite  $\alpha\nu$  fermions labeled by the indices  $\alpha = \eta, s$  and  $\nu = 1, 2, \dots$ , and a well-defined number of independent  $\eta$ -spinons and independent spinons. The latter objects are invariant under the above unitary transformation and thus have a non-interacting character for  $U/4t > 0$ . The composite  $\alpha\nu$  fermions and corresponding  $\alpha\nu$  bond particles involve  $2\nu$   $\eta$ -spinons ( $\alpha = \eta$ ) or  $2\nu$  spinons ( $\alpha = s$ ) where  $\nu = 1, 2, \dots$  is the number of  $\eta$ -spin-neutral  $\eta$ -spinon (and spin-neutral spinon) pairs.

##### A. The composite $\alpha\nu$ bond particles and $\alpha\nu$ fermions

###### 1. The $\alpha\nu$ fermion operators and $\alpha\nu$ translation generators

Alike for the  $s1$  bond particles further studied in Refs.<sup>1,18</sup>, one can introduce within the  $N_a^D \rightarrow \infty$  limit suitable creation operators  $g_{\vec{r}_j, \alpha\nu}^\dagger$  for the  $\alpha\nu$  bond particles. Provided that  $(1 - x) > 0$  for  $\alpha\nu = s1$  and  $S_\alpha/N_a^D > 0$  for the remaining  $\alpha\nu$  branches, the  $\alpha\nu$  bond-particle operators have been constructed to inherently upon acting onto their  $\alpha\nu$  effective lattice introduced below in Subsection IV-D anticommute on the same site and commute on different sites, so that they are hard-core like and can be transformed onto fermionic operators whose general expression reads,

$$f_{\vec{r}_j, \alpha\nu}^\dagger = e^{i\phi_{j, \alpha\nu}} g_{\vec{r}_j, \alpha\nu}^\dagger; \quad \phi_{j, \alpha\nu} = \sum_{j' \neq j} f_{\vec{r}_{j'}, \alpha\nu}^\dagger f_{\vec{r}_{j'}, \alpha\nu} \phi_{j', j, \alpha\nu}; \quad \phi_{j', j, \alpha\nu} = \arctan \left( \frac{x_{j'2} - x_{j2}}{x_{j'1} - x_{j1}} \right),$$

$$f_{\vec{q}_j, \alpha\nu}^\dagger = \frac{1}{\sqrt{N_{a\alpha\nu}^D}} \sum_{j'=1}^{N_{a\alpha\nu}^D} e^{+i\vec{q}_j \cdot \vec{r}_{j'}} f_{\vec{r}_{j'}, \alpha\nu}^\dagger, \quad (1 - x) > 0 \text{ for } \alpha\nu = s1 \text{ and } S_\alpha/N_a^D > 0 \text{ for } \alpha\nu \neq s1. \quad (24)$$

Here  $\phi_{j,\alpha\nu}$  is the Jordan-Wigner phase<sup>20</sup> operator, the indices  $j'$  and  $j$  refer to sites of the  $\alpha\nu$  effective lattice, and  $f_{\vec{q}_j,\alpha\nu}^\dagger$  are the corresponding momentum-dependent  $\alpha\nu$  fermion operators. The number  $N_{a_{\alpha\nu}}^D$  of discrete momentum values of the  $\alpha\nu$  momentum band equals that of sites of the  $\alpha\nu$  effective lattice derived below in Subsection IV-D. In turn, if for  $\alpha\nu \neq s1$  branches one has that  $S_\alpha = 0$  and  $N_{\alpha\nu}/N_a^D \ll 1$ , provided that  $N_{\alpha\nu'} = 0$  for all remaining  $\alpha\nu'$  branches with a number of  $\eta$ -spinon or spinon pairs  $\nu' > \nu$  one finds below that  $N_{a_{\alpha\nu}}^D = N_{\alpha\nu}$ , the phase operator  $\phi_{j,\alpha\nu}$  may be replaced by the average phase  $\phi_{j,\alpha\nu} \approx \phi_{j,\alpha\nu}^0 = \sum_{j' \neq j} \phi_{j',j,\alpha\nu}$ , and the momenta of the operators  $f_{\vec{q}_j,\alpha\nu}^\dagger$  are given by  $\vec{q}_j \approx 0$ . In the latter case all sites of the  $\alpha\nu$  effective lattice are occupied and the  $\alpha\nu$  momentum band is full. If the value of  $N_{\alpha\nu}$  is finite one has  $N_{a_{\alpha\nu}}^D = N_{\alpha\nu}$  discrete momentum values  $\vec{q}_j \approx 0$  distributed around zero momentum, whose Cartesian components momentum spacing is  $2\pi/L$ . A case of interest is when  $N_{\alpha\nu} = 1$  so that the  $\alpha\nu$  effective lattice has a single site and the corresponding  $\alpha\nu$  band a single discrete momentum value,  $\vec{q} = 0$ . In that case  $\phi_{\alpha\nu} = \phi_{j,\alpha\nu} = 0$  so that  $f_{\vec{r},\alpha\nu}^\dagger = g_{\vec{r},\alpha\nu}^\dagger$  and  $f_{\vec{q},\alpha\nu}^\dagger = f_{\vec{r},\alpha\nu}^\dagger$  where  $\vec{q} = 0$ .

As further discussed in Subsection IV-E, the operators  $f_{\vec{q}_j,\alpha\nu}^\dagger$  act onto subspaces with constant values for the set of numbers  $S_\alpha$ ,  $N_{\alpha\nu}$ , and  $\{N_{\alpha\nu'}\}$  for  $\nu' > \nu$  and equivalently of the numbers  $S_c$ ,  $N_{\alpha\nu}$ , and  $\{N_{\alpha\nu'}\}$  for all  $\nu' \neq \nu$ . Such subspaces are spanned by mutually neutral states, that is states with constant values for the numbers of  $\alpha\nu$  fermions and  $\alpha\nu$  fermion holes, respectively. Hence such states can be transformed into each other by  $\alpha\nu$  band particle-hole processes. The phases  $\phi_{j,\alpha\nu}$  given in Eq. (24) are associated with an effective vector potential<sup>20,36</sup>,

$$\begin{aligned} \vec{A}_{\alpha\nu}(\vec{r}_j) &= \Phi_0 \sum_{j' \neq j} n_{\vec{r}_{j'},\alpha\nu} \frac{\vec{e}_{x3} \times (\vec{r}_{j'} - \vec{r}_j)}{(\vec{r}_{j'} - \vec{r}_j)^2}; \quad n_{\vec{r}_j,\alpha\nu} = f_{\vec{r}_j,\alpha\nu}^\dagger f_{\vec{r}_j,\alpha\nu}, \\ \vec{B}_{\alpha\nu}(\vec{r}_j) &= \vec{\nabla}_{\vec{r}_j} \times \vec{A}_{\alpha\nu}(\vec{r}_j) = \Phi_0 \sum_{j' \neq j} n_{\vec{r}_{j'},\alpha\nu} \delta(\vec{r}_{j'} - \vec{r}_j) \vec{e}_{x3}; \quad \Phi_0 = 1, \end{aligned} \quad (25)$$

where  $\vec{e}_{x3}$  is the unit vector perpendicular to the plane and we use units such that the fictitious magnetic flux quantum is given by  $\Phi_0 = 1$ . It follows from the form of the effective vector potential  $\vec{A}_{\alpha\nu}(\vec{r}_j)$  that the present description leads to the intriguing situation where the  $\alpha\nu$  fermions interact via long-range forces while all interactions in the original Hamiltonian are onsite.

The components of the microscopic momenta of the  $\alpha\nu$  fermions are eigenvalues of the two (and one for 1D)  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu x_1}$  and  $\hat{q}_{\alpha\nu x_2}$  in the presence of the fictitious magnetic field  $\vec{B}_{\alpha\nu}(\vec{r}_j)$ . That seems to imply that for the model on the square lattice the components  $q_{x1}$  and  $q_{x2}$  of the microscopic momenta  $\vec{q} = [q_{x1}, q_{x2}]$  refer to operators that do not commute. However, such operators commute in the subspaces where the operators  $f_{\vec{q}_j,\alpha\nu}^\dagger$  act onto because those are spanned by neutral states<sup>36</sup>. Since  $[\hat{q}_{\alpha\nu x_1}, \hat{q}_{\alpha\nu x_2}] = 0$  in such subspaces, for the model on the square lattice the  $\alpha\nu$  fermions carry a microscopic momentum  $\vec{q} = [q_{x1}, q_{x2}]$  where the components  $q_{x1}$  and  $q_{x2}$  are well-defined simultaneously. Importantly, it follows that the momentum operator  $\hat{\vec{P}}$  of Eq. (5) commutes with the  $\alpha\nu$  generators  $\hat{q}_{\alpha\nu}$  whose eigenvalues are the  $\alpha\nu$  fermion microscopic momenta  $\vec{q}$ . Hence, within our description the momentum operator (5) can be written as,

$$\hat{\vec{P}} = \hat{\vec{q}}_c + \sum_{\nu=1}^{Cs} \hat{\vec{q}}_{s\nu} + \sum_{\nu=1}^{C\eta} \hat{\vec{q}}_{\eta\nu} + \vec{\pi} \hat{M}_{\eta,-1/2}, \quad (26)$$

where the  $c$  and  $\alpha\nu$  translation generators read,

$$\hat{\vec{q}}_c = \sum_{\vec{q}} \vec{q} \hat{N}_c(\vec{q}); \quad \hat{\vec{q}}_{s\nu} = \sum_{\vec{q}} \vec{q} \hat{N}_{s\nu}(\vec{q}); \quad \hat{\vec{q}}_{\eta\nu} = \sum_{\vec{q}} [\vec{\pi} - \vec{q}] \hat{N}_{\eta\nu}(\vec{q}). \quad (27)$$

Here  $\vec{\pi}$  is the momentum carried by a  $-1/2$   $\eta$ -spinon, the operator  $\hat{M}_{\eta,-1/2}$  counts the number  $M_{\eta,-1/2} = [L_{\eta,-1/2} + C_\eta]$  of such objects, that the  $\eta\nu$  generators involve  $[\vec{\pi} - \vec{q}]$  instead of  $\vec{q}$  follows from the anti-bounding character of the  $\eta\nu$  fermions discussed below, and  $\hat{N}_c(\vec{q})$  and  $\hat{N}_{\alpha\nu}(\vec{q})$  are the momentum distribution-function operators,

$$\hat{N}_c(\vec{q}) = f_{\vec{q},c}^\dagger f_{\vec{q},c}; \quad \hat{N}_{\alpha\nu}(\vec{q}) = f_{\vec{q},\alpha\nu}^\dagger f_{\vec{q},\alpha\nu}, \quad (28)$$

respectively.

For the Hubbard model both on the square and 1D lattices the Hamiltonian  $\hat{H}$  of Eq. (1) and the momentum operator  $\hat{\vec{P}}$  of Eqs. (5) and (26) obey the commutation relations,

$$[\hat{H}, \hat{\vec{P}}] = [\hat{H}, \hat{M}_{\alpha,\pm 1/2}] = [\hat{H}, \hat{\vec{q}}_c] = 0; \quad [\hat{\vec{P}}, \hat{M}_{\alpha,\pm 1/2}] = [\hat{\vec{P}}, \hat{\vec{q}}_c] = [\hat{\vec{P}}, \hat{\vec{q}}_{\alpha\nu}] = 0, \quad (29)$$

for  $\nu = 1, \dots, C_\alpha$  and  $\alpha = \eta, s$ . In turn, the set of commutators  $[\hat{H}, \hat{q}_{\alpha\nu}]$  vanish for the 1D model whereas for the model on the square lattice one has in general that  $[\hat{H}, \hat{q}_{\alpha\nu}] \neq 0$ . It follows from Eq. (26) that the momentum eigenvalues  $\vec{P}$  can be expressed as a sum of the filled  $c$  and  $\alpha\nu$  fermion microscopic momenta.

In the limit  $N_a \rightarrow \infty$  one has that  $\sum_{\alpha=\eta,s} C_\alpha \rightarrow \infty$  for most subspaces so that the set of  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu}$  of Eq. (27) in the presence of the fictitious magnetic fields  $\vec{B}_{\alpha\nu}$  of Eq. (25) is infinite. That for 1D all such operators commute both with the Hamiltonian and momentum operator is behind the integrability of the 1D Hubbard model in that limit. Indeed, such an infinite set of translation generators is equivalent to the infinite set of conservation laws, which are known to be behind that model integrability<sup>16,46</sup>. Such laws are also equivalent to the conservation of the set of  $\alpha\nu$  fermion numbers  $\{N_{\alpha\nu}\}$  where  $\alpha = \eta, s$ ,  $\nu = 1, \dots, C_\alpha$  and the maximum  $C_\alpha$  magnitude is  $N_a^D/2$  and thus  $N_a/2$  for 1D<sup>46</sup>. In turn, the Hubbard model on the square lattice is not integrable and consistently the set of  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu}$  of Eq. (27) do not commute in general with the Hamiltonian so that the corresponding  $\alpha\nu$  fermion discrete momentum values  $\vec{q}_j = [q_{x1}, q_{x2}]$  are not good quantum numbers. As further discussed in Subsection IV-E, that as given in Eq. (29) for the square-lattice model such  $\alpha\nu$  translation generators commute with momentum operator is consistent with it being invariant under the electron - rotated-electron unitary transformation and the  $\alpha\nu$  fermion operators acting onto subspaces spanned by mutually neutral states. In general such subspaces refer to constant values of the number of  $\alpha\nu$  fermions.

It turns out that processes within the one- and two-electron subspace as defined in this paper where two  $s1$  fermions are annihilated and one  $s2$  fermion created are also neutral in the sense that for the model on the square lattice the  $s1$  fermion microscopic momenta  $\vec{q} = [q_{x1}, q_{x2}]$  are for such excitations associated with  $s1$  translation generators  $\hat{q}_{s1\ x1}$  and  $\hat{q}_{s1\ x2}$  that commute. Moreover, in such a subspace there are no  $\alpha\nu$  fermions other than  $s1$  fermions and none or one zero-momentum  $s2$  fermion. The interest of our operator description lies in that for the Hubbard model on the square lattice in the neutral subspaces of the one- and two-electron subspace the  $s1$  translation generators  $\hat{q}_{s1}$  of Eq. (27) in the presence of the fictitious magnetic field  $\vec{B}_{s1}$  commuting with both the Hamiltonian and momentum operator. As justified below, in spite of the lack of the square-lattice model integrability, for that model in such a subspace the  $s1$  translation generators have been constructed to inherently these commutation relations holding. Therefore, for the square-lattice quantum liquid corresponding to the Hubbard model on a square lattice in the one- and two-electron subspace as defined in this paper the  $s1$  fermion discrete momentum values  $\vec{q} = [q_{x1}, q_{x2}]$  are good quantum numbers and thus are conserved. We emphasize that according to Eq. (29) the commutator  $[\hat{H}, \hat{q}_c]$  vanishes so that for the model on the square lattice the  $c$  band momenta are good quantum numbers for the whole Hilbert space, alike for the 1D model. Hence for the model on the square lattice in the one- and two-electron subspace both the  $c$  band and  $s1$  band discrete momentum values are good quantum numbers. This result follows from the way that our operator description is constructed. However, the shape of the  $s1$  momentum band and of its boundary as well as the form of the  $s1$  and  $c$  fermion energy dispersions remain unsolved problems, which are addressed in Ref.<sup>1</sup>.

The advantage of using momentum-dependent  $c$  fermion operators  $f_{\vec{q}_j, c}^\dagger$  and  $\alpha\nu$  fermion operators  $f_{\vec{q}_j, \alpha\nu}^\dagger$  given in Eqs. (8) and (24), respectively, is then that for the 1D model in the whole Hilbert space and the model on the square lattice in the one- and two-electron subspace as defined in this paper such microscopic momenta are good quantum numbers. That for the model on the square lattice the  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu}$  of Eq. (27) in the presence of the fictitious magnetic field  $\vec{B}_{\alpha\nu}$  do not commute in general with the Hamiltonian is consistent with the set of  $\alpha\nu$  fermion numbers  $\{N_{\alpha\nu}\}$  which label the  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates considered in Subsection IV-E not being in general good quantum numbers.

The related studies of Refs.<sup>1,22</sup> focus mainly on the square-lattice quantum liquid in the one- and two-electron subspace. In turn, here we consider as well general  $\mathcal{N}$ -electron subspaces where  $\mathcal{N} = 1, 2, 3, 4, \dots$ . The  $\alpha\nu$  fermion operators  $f_{\vec{q}, \alpha\nu}^\dagger$  and  $f_{\vec{q}, \alpha\nu}$  act onto subspaces spanned by neutral states. Nevertheless, creation of one  $\alpha\nu$  fermion is a well-defined process whose generator is the product of an operator, which fulfills small changes in the  $\alpha\nu$  effective lattice and corresponding  $\alpha\nu$  momentum band and the operator  $f_{\vec{q}, \alpha\nu}^\dagger$  appropriate to the excited-state subspace. It turns out that for the model on the 1D and square lattices creation of one  $\eta\nu$  fermion onto a  $[N_a^2 - N] = 2\nu$  ground state generates for  $U/4t > 0$  a  $2\nu$ -electron charge excited energy eigenstate. Moreover, creation of one  $s\nu$  fermion onto a  $[N_\uparrow - N_\downarrow] = 2\nu$  ground state generates a  $2\nu$ -electron spin excited energy eigenstate. Furthermore and as discussed below in Subsection IV-E, the created  $\eta\nu$  fermion or  $s\nu$  fermion is invariant under the electron - rotated-electron unitary transformation. However, the detailed internal structure of the composite  $\alpha\nu$  fermions is in general a unsolved complex problem.

Since the microscopic momenta of the  $c$  fermions are good quantum numbers for the model on the square lattice, one can define an energy dispersion  $\epsilon_c(\vec{q})$ <sup>1</sup>. For the 1D model the  $\alpha\nu$  energy dispersions  $\epsilon_{\alpha\nu}(\vec{q})$  are well defined as well. In turn, for the model on the square lattice the energies  $\epsilon_{\alpha\nu}(\vec{q})$  have for  $\alpha\nu \neq s1$  no uncertainty for the momentum values for which such objects are invariant under the electron - rotated-electron unitary transformation. This is the case of the above  $\eta\nu$  fermion created onto a  $[N_a^2 - N] = 2\nu$  ground state and  $s\nu$  fermion onto a  $[N_\uparrow - N_\downarrow] = 2\nu$  ground

state whose excited-state  $\alpha\nu$  momentum band corresponds to the zero momentum value only, as confirmed below. For general  $\alpha\nu$  fermion momentum values there is some uncertainty in the magnitude of  $\epsilon_{\alpha\nu}(\vec{q})$  yet fortunately it refers to a well-defined energy window. There is in general a uncertainty in the magnitude of  $\epsilon_{s1}(\vec{q})$  as well yet such an energy dispersion is well defined for the one- and two-electron subspace<sup>1</sup>.

Within our  $N_a^D \gg 1$  limit one can access general useful information on the energies  $\epsilon_c$  and  $\epsilon_{\alpha\nu}$  without knowing in detail the form of the  $\alpha\nu$  bond-particle operators  $g_{\vec{r}_j, \alpha\nu}^\dagger$  and corresponding  $\alpha\nu$  fermion operators  $f_{\vec{r}_j, \alpha\nu}^\dagger$ , which for  $\alpha = \eta$  (and  $\alpha = s$ ) involve a set of  $\eta$ -spinon operators  $p_{\vec{r}_j}^l = (1 - n_{\vec{r}_j, c}) q_{\vec{r}_j}^l$  (and spinon operators  $s_{\vec{r}_j}^l = n_{\vec{r}_j, c} q_{\vec{r}_j}^l$ ) given in Eqs. (9)-(11) associated with the  $\eta$ -spin (and spin) neutral superposition of the corresponding  $2\nu = 2, 4, 6, \dots$   $\eta$ -spinons (and spinons). (The  $s1$  bond-particle operators  $g_{\vec{r}_j, s1}^\dagger$  are studied in Ref.<sup>18</sup>.) Since as confirmed below, the ground-state occupancy configurations involve only the charge  $c$  fermions and composite two-spinon  $s1$  fermions, that problem is addressed for the one- and two-electron subspace in Refs.<sup>1,22</sup> concerning the  $s1$  fermions. The studies of such references profit from the  $c$  fermions and  $s1$  fermions being the only objects playing an active role in that subspace. In turn, in the following we access general information about such composite objects including for instance the anti-bounding and bounding character of the  $2\nu$ - $\eta$ -spinon composite  $\eta\nu$  fermions and  $2\nu$ -spinon composite  $s\nu$  fermions, respectively, and the energy uncertainty of their energy spectrum, which is smaller than or equals the corresponding energy bandwidth. For the Hubbard model on the square lattice in the one- and two-electron subspace such objects play the role of “quasiparticles”. Due to integrability, for the 1D model they have zero-momentum forward-scattering interactions only. In turn, for the model on the square lattice the unusual scattering properties of the quantum problem are controlled and determined by the inelastic  $c$  -  $s1$  fermion collisions<sup>32</sup>.

For the limit  $N_a^D \gg 1$  considered in this paper the problem of the internal degrees of freedom of the composite  $\alpha\nu$  fermions separates from that of their positions in the corresponding  $\alpha\nu$  effective lattice defined below and corresponding discrete momentum values in the  $\alpha\nu$  band, whose number equals that of sites in such a lattice. In this section it is confirmed that for the subspaces spanned by states with constant values of  $S_\eta$ ,  $S_s$ , and  $S_c$  the momentum occupancy configurations of the composite  $\alpha\nu$  fermions and  $c$  fermions generate the correct number of state configurations of the group  $SO(3) \times SO(3) \times U(1)$ . Addition of the dimensions of all such subspaces leads to a total number  $4^{N_a^2}$  of independent state representations, which indeed is the dimension of the Hilbert space. Furthermore, we initiate the study of the  $c$  and  $s1$  effective lattices for the states that span the one- and two-electron subspace as defined in this paper.

For the particular case of the 1D Hubbard model, a preliminary version of the general operator description introduced here for both the model on the square and 1D lattices is presented in Ref.<sup>37</sup>. The studies of that reference profit from the exact solution of the 1D model. No explicit relations to the rotated-electron operators as those given in Eqs. (8)-(17) are derived and no relation to the  $U(1)$  symmetry contained in the model  $SO(3) \times SO(3) \times U(1)$  global symmetry is established. Indeed, the eigenvalue of the generator (7) of the  $U(1)$  symmetry is one half the number of rotated-electron singly occupied sites  $2S_c$ . Such an eigenvalue plays an important role in the present description. It determines the values of the number  $N_c = 2S_c$  of  $c$  fermions,  $M_s = 2S_c$  of spinons,  $N_c^h = [N_a^D - 2S_c]$  of  $c$  fermion holes, and  $M_\eta = [N_a^D - 2S_c]$  of  $\eta$ -spinons. In reference<sup>37</sup> the  $\eta$ -spinons,  $c$  fermions, independent  $\eta$ -spinons, and independent spinons are called holons,  $c$  pseudoparticles, Yang holons, and HL spinons, respectively, where HL stands for Heilmann and Lieb. Moreover, the  $\alpha\nu$  pseudoparticles considered in that reference are the  $\alpha\nu$  fermions.

## 2. More about the states representation in terms of composite $\alpha\nu$ fermion occupancy configurations

For the model (1) on the square lattice the sites of the  $\eta$ -spin (and spin) effective lattice are distributed along well-defined  $ox_1$  and  $ox_2$  directions, defined by the fundamental vectors  $\vec{a}_{x_1} = a \vec{e}_{x_1}$  and  $\vec{a}_{x_2} = a \vec{e}_{x_2}$  of the original lattice where  $\vec{e}_{x_1}$  and  $\vec{e}_{x_2}$  are the usual Cartesian unit vectors and  $a$  is the lattice constant. The average distance between such sites when going through these directions is  $a_\alpha = L/N_{a_\alpha} = [N_a/N_{a_\alpha}]a$  where  $\alpha = \eta, s$ . For 1D this is also the average distance between the sites of such effective lattices.  $a_\eta$  is the average distance along the  $ox_1$  and/or the  $ox_2$  direction between the sites that are either doubly occupied or unoccupied by rotated electrons.  $a_s$  is the average distance along that and/or those directions between the sites that are singly occupied by rotated electrons.

The concept of a  $\eta$ -spin (and spin) effective lattice is well defined for finite values of the hole concentration  $x$  (and electronic density  $n = (1 - x)$ ) and the present  $N_a^D \gg 1$  limit. The general representation introduced in this paper contains full information about the relative positions of the sites of the  $\eta$ -spin and spin effective lattices in the original lattice. For each rotated-electron occupancy configuration that generates a given momentum eigenstate, such an information is stored in the corresponding occupancy configurations of the  $c$  fermions in their  $c$  effective lattice, which is identical to the original lattice. The latter configurations correspond to the state representations of the  $U(1)$  symmetry in the subspaces spanned by states with constant values of  $S_c$ ,  $S_\eta$ , and  $S_s$ . Indeed, the sites of the  $\eta$ -spin (and spin) effective lattice have in the original lattice the same real-space coordinates as the sites of

the  $c$  effective lattice unoccupied (and occupied) by  $c$  fermions. That such an information is stored in the  $c$  fermion occupancy configurations is consistent with the  $\eta$ -spinon and spinon occupancy configurations of the  $\eta$ -spin and spin effective lattices, respectively, being independent of each other. The latter occupancy configurations refer to the state representations of the  $SU(2)$   $\eta$ -spin and spin symmetries, respectively, in the subspaces with constant values of  $S_c$ ,  $S_\eta$ , and  $S_s$ .

For the model on the 1D lattice the  $\eta$ -spin (and spin) effective lattice is straightforwardly and uniquely obtained by considering only the rotated-electron doubly and unoccupied sites (and singly occupied sites) of the original lattice and keeping the same site order as for that lattice. In turn, for the model on the square lattice the  $\eta$ -spin (and spin) effective lattice is in the limit  $x \rightarrow 1$  (and  $x \rightarrow 0$ ) exactly a square lattice. Indeed, in that limit it becomes identical to the original lattice. Moreover, it is an excellent approximation to consider that for small electron density  $n = (1 - x)$  (and small hole concentration  $x$ ) the  $\eta$ -spin (and spin) effective lattice is a square lattice.

Since the  $\eta$ -spinon, spinon, and  $c$  fermion description contains full information about the relative positions of the sites of the  $\eta$ -spin and spin effective lattices in the original lattice, it turns out that within the  $N_a^D \gg 1$  limit and for finite values of the hole concentration  $x$  (and electron density  $n = (1 - x)$ ) the  $\eta$ -spin (and spin) effective lattice can for 2D be represented by a square lattice with lattice constant  $a_\eta$  (and  $a_s$ ) given by,

$$a_\alpha = \frac{L}{N_{a_\alpha}} = \frac{N_a}{N_{a_\alpha}} a; \quad \alpha = \eta, s. \quad (30)$$

The expression of the operator  $\hat{S}$  such that  $\hat{V}^\dagger = e^{\hat{S}}$  and  $\hat{V} = e^{-\hat{S}}$  involves only the three kinetic operators  $\hat{T}_0$ ,  $\hat{T}_{+1}$ , and  $\hat{T}_{-1}$  given in Eq. (2). Therefore, when expressed in terms of rotated-electron creation and annihilation operators the expression of the electron - rotated-electron unitary operator  $\hat{V} = \tilde{V} = e^{-\hat{S}}$  involves only the corresponding three rotated kinetic operators  $\tilde{T}_0$ ,  $\tilde{T}_{+1}$ , and  $\tilde{T}_{-1}$  and thus preserves the occurrence of only nearest hopping for rotated electrons, alike for electrons. Indeed, the effective rotated-electron hopping between second and third nearest neighboring sites is generated by products of such operators so that the corresponding elementary hopping processes correspond only to nearest hopping. This confirms that in the square lattice the rotated electrons hop along the  $ox_1$  or the  $ox_2$  direction between the sites. Hence the same holds for  $\eta$ -spinons (and spinons) moving in the corresponding  $\eta$ -spin and spin effective lattices, consistently with those being square lattices.

The  $\eta$ -spin (and spin) effective lattice includes only the rotated-electron doubly and unoccupied sites (and singly occupied sites) of the original lattice. However, within periodic boundary conditions a pair of rotated electrons or rotated holes (and a rotated electron) moving once around the chain in 1D and through the whole crystal along the  $ox_1$  or  $ox_2$  directions in the square lattice and doubly occupying (and singly occupying) a site in each step must pass an overall distance  $L$ . Therefore, consistently with expression  $a_\alpha = L/N_{a_\alpha} = [N_a/N_{a_\alpha}]a$  introduced below where  $\alpha = \eta, s$ , the  $\eta$ -spin (and spin) effective lattice has both for 1D and 2D the same length and edge length  $L$ , respectively, as the original lattice. Furthermore, the requirement that for the 2D case when going through the whole crystal along the  $ox_1$  or  $ox_2$  directions a  $\eta$  spinon (and spinon) passes an overall distance  $L$  is met by a square effective  $\eta$ -spin (and spin) lattice. However, since the number of sites sum-rule  $[N_{a_\eta}^D + N_{a_s}^D] = N_a^D$  holds, the  $\eta$ -spin and spin effective lattices have in general a number of sites  $N_{a_\alpha}^D$  smaller than that of the original lattice,  $N_a^D$ . It follows that their lattice constants given in Eq. (30) are larger than that of the original lattice,  $a_\alpha \geq a$  where  $\alpha = \eta, s$ .

The average distance between the sites of the  $\eta$ -spin and spin effective lattices provided in that equation then plays the role of lattice constant of such lattices. The validity for  $N_a^D \gg 1$  of the square spin effective lattice constructed in that way is confirmed by the average value  $\langle \Psi | \delta d | \Psi \rangle$  relative to any energy eigenstate  $|\Psi\rangle$  belonging to a subspace with constant number of rotated-electron singly occupied sites of the distance  $\delta d$  in real space of any of the  $N_{a_s}^D$  sites of the spin effective lattice from the rotated-electron singly occupied site of the original lattice closest to it vanishing in the limit  $N_a^D \rightarrow \infty$ . We recall that the number of rotated-electron singly occupied sites of the original lattice equals that of sites of the spin effective lattice.

It is useful to consider the occupancy configurations of the  $2S_\eta$  (and  $2S_s$ ) "unoccupied sites" and the  $2C_\eta$  (and  $2C_s$ ) "occupied sites" of the  $\eta$ -spin (and spin) effective lattice that generate state representations of the model global  $SO(3) \times SO(3) \times U(1)$  symmetry. For the LWS-subspace considered here the  $2S_\eta$  (and  $2S_s$ ) "unoccupied sites" of such a lattice correspond to  $2S_\eta$  independent  $+1/2$   $\eta$ -spinons (and  $2S_s$  independent  $+1/2$  spinons) that remain invariant under the unitary transformation associated with the operator  $\hat{V}$ . In turn, the  $C_\eta + 1/2$   $\eta$ -spinons and  $C_\eta - 1/2$   $\eta$ -spinons (and  $C_s + 1/2$  spinons and  $C_s - 1/2$  spinons) that refer to the  $2C_\eta$  (and  $2C_s$ ) "occupied sites" of such a lattice do not remain invariant under that unitary transformation.

From the relation of the transformation laws under the electron - rotated-electron unitary transformation to the number of  $\eta$ -spin (and spin) singlet configurations of the subspaces with constant values of  $S_c$ ,  $S_\eta$ , and  $S_s$  one finds that such configurations can be expressed in terms of occupancies of  $\eta$ -spin-neutral  $2\nu$ - $\eta$ -spinon composite  $\eta\nu$  bond particles (and spin-neutral  $2\nu$ -spinon composite  $s\nu$  bond particles) in suitable and independent  $\eta\nu$  effective lattices (and  $s\nu$  effective lattices). We recall that here  $\nu = 1, 2, \dots, C_\eta$  (and  $\nu = 1, 2, \dots, C_s$ ) is the number of  $\eta$ -spinon pairs



(and spinon pairs) of opposite  $\eta$ -spin projection (and spin projection) in each composite  $\eta\nu$  bond particle (and  $s\nu$  bond particle). Among such composite  $\alpha\nu$  bond particles, the two-spinon  $s1$  bond particles play a major role since they are found below to be the only of the composite objects with finite occupancy in the ground states. Such two-spinon objects are found in Ref.<sup>18</sup> to be related to the resonating-valence-bond pictures considered long ago<sup>34,38-40</sup> for spin-singlet occupancy configurations of ground states.

The  $\alpha\nu$  fermions have the same internal structure as the corresponding  $\alpha\nu$  bond particles and live on the  $\alpha\nu$  effective lattice as well. Hence a  $\eta\nu$  fermion (and  $s\nu$  fermion) is a  $\eta$ -spin-neutral  $2\nu$ - $\eta$ -spinon composite (and spin-neutral  $2\nu$ -spinon composite) object. Since within our description the momentum occupancy configurations of the  $c$  and  $\alpha\nu$  fermions generate momentum eigenstates, in the following we refer mostly to  $\alpha\nu$  fermions, yet many of our considerations apply as well to the corresponding  $\alpha\nu$  bond particles. Indeed, as given in Eq. (24) the creation operator  $f_{\vec{r}_j,\alpha\nu}^\dagger$  of a local  $\alpha\nu$  fermion of real-space coordinate  $\vec{r}_j$  differs from the creation operator  $g_{\vec{r}_j,\alpha\nu}^\dagger$  of the corresponding  $\alpha\nu$  bond particle with the same real-space coordinate by a phase factor  $e^{i\phi_{j,\alpha\nu}}$ ,  $f_{\vec{r}_j,\alpha\nu}^\dagger = e^{i\phi_{j,\alpha\nu}} g_{\vec{r}_j,\alpha\nu}^\dagger$ . Otherwise, such objects have the same internal structure.

Our description is consistent with the Abelian and non-Abelian character of the  $U(1)$  symmetry and two  $SU(2)$  symmetries, respectively, of the model global  $[SU(2) \times SU(2) \times U(1)]/Z_2^2 = SO(3) \times SO(3) \times U(1)$  symmetry. Indeed, the  $c$  fermions occupancy configurations refer to the state representations of a  $U(1)$  symmetry associated with an Abelian group and hence involve a single  $c$  effective lattice. In contrast, the  $\eta$ -spinon (and spinon) occupancy configurations refer to the state representations of a  $SU(2)$  symmetry associated with a non-Abelian group so that several types of  $\eta$ -spin (and spin) singlet configurations emerge, each corresponding to a  $\eta\nu$  effective lattice (and  $s\nu$  effective lattice) occupied by  $\eta$ -spin-zero (and spin-zero) composite objects of  $2\nu$   $\eta$ -spinons (and  $2\nu$  spinons). As confirmed below, there exists an independent  $\alpha\nu$  effective lattice for each  $\alpha\nu$  branch where  $\alpha = \eta, s$  and  $\nu = 1, \dots, C_\alpha$ . Here  $\alpha$  refers to  $\eta$ -spin ( $\alpha = \eta$ ) and spin ( $\alpha = s$ ) and  $\nu$  to the number of  $\eta$ -spin-singlet  $\eta$ -spinon pairs ( $C_\alpha = C_\eta$ ) and spin-singlet spinon pairs ( $C_\alpha = C_s$ ).

Within chromodynamics the quarks have color but all quark-composite physical particles are color-neutral<sup>41</sup>. Here the  $\eta$ -spinon (and spinons) that are not invariant under the electron - rotated-electron unitary transformation have  $\eta$  spin  $1/2$  (and spin  $1/2$ ) but are part of  $\eta$ -spin-neutral (and spin-neutral)  $2\nu$ - $\eta$ -spinon (and  $2\nu$ -spinon) composite  $\eta\nu$  fermions (and  $s\nu$  fermions). The occurrence of such  $\eta$ -spin neutral  $\eta\nu$  fermions (and spin neutral  $s\nu$  fermions) leads to the following expression for the number  $2C_\alpha$  of "occupied sites" of the  $\eta$ -spin ( $\alpha = \eta$ ) and spin ( $\alpha = s$ ) effective lattice of Eq. (20), which refers to the subspaces spanned by states with constant values of  $S_c$ ,  $S_\eta$ , and  $S_s$ ,

$$2C_\alpha = 2 \sum_{\nu=1}^{C_\alpha} \nu N_{\alpha\nu}; \quad N_{a_\alpha}^D = M_\alpha = 2S_\alpha + 2C_\alpha; \quad \alpha = \eta, s. \quad (31)$$

Here  $N_{\alpha\nu}$  denotes the number of composite  $\alpha\nu$  fermions. Each subspace spanned by states with constant values of  $S_c$ ,  $S_\eta$ , and  $S_s$  and hence also with constant values of  $C_\eta$  and  $C_s$  can be divided into smaller subspaces spanned by states with constant values for the set of numbers  $\{N_{\eta\nu}\}$  and  $\{N_{s\nu}\}$ , which must obey the sum rules of Eq. (31). The numbers  $\{N_{\eta\nu}\}$  and  $\{N_{s\nu}\}$  correspond to operators that commute with the momentum operator and operators associated with the numbers  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ , and  $S_c$ . In turn, for the model on the square lattice such operators do not commute with the Hamiltonian so that the numbers  $\{N_{\eta\nu}\}$  and  $\{N_{s\nu}\}$  are not in general good quantum numbers. The same applies to the set of  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu}^\dagger$  of Eq. (27) in the presence of the fictitious magnetic field  $\vec{B}_{\alpha\nu}$  of Eq. (25), which as given in Eq. (29) commute with the momentum operator yet in general do not commute with the Hamiltonian of the model on the square lattice. For 1D both such  $\alpha\nu$  translation generators commute with the Hamiltonian and the set of numbers  $\{N_{\alpha\nu}\}$  are within our limit  $N_a^D \rightarrow \infty$  associated with the set of conservation laws behind the model integrability<sup>46</sup> and thus are conserved. Fortunately, we confirm below that they are good quantum numbers as well for the model on the square lattice in the one- and two-electron subspace and read  $N_{\eta\nu} = 0$ ,  $N_{s1} = [S_c - S_s - 2N_{s2}]$ ,  $N_{s2} = 0, 1$ , and  $N_{s\nu} = 0$  for  $\nu \geq 3$ , consistently with and the  $s1$  translation generator  $\hat{q}_{s1}^\dagger$  of Eq. (27) in the presence of the fictitious magnetic field  $\vec{B}_{s1}$  of Eq. (25) commuting with both the Hamiltonian and momentum operator.

In the following we consider the complete set of  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates also labelled by the numbers  $\{N_{\eta\nu}\}$  and  $\{N_{s\nu}\}$ . The expressions of the corresponding  $\alpha\nu$  fermion operators involve the spinon ( $\alpha = s$ ) and  $\eta$ -spinon ( $\alpha = \eta$ ) operators of Eqs. (9), (10), and (11). Both such spinon and  $\eta$ -spinon operators and the  $c$  fermion operators are expressed in terms of the rotated-electron operators given in Eq. (8), which are generated from the corresponding electron operators by the electron - rotated-electron unitary operator as defined in this paper. Hence and as discussed below in subsection IV-E, for the model on the square lattice both the present  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates and the unknown energy eigenstates are generated by application onto the corresponding sets of  $U/4t \rightarrow \infty$  states by the same electron - rotated-electron unitary operator  $\hat{V}^\dagger = \hat{V}^\dagger(U/4t)$ . Indeed, for that model the energy eigenstates are a superposition of a set of the former  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates

with the same momentum and  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ , and  $S_c$  values. For the 1D model both sets of states are identical, due to the infinite conservation laws, which for  $N_a^D \rightarrow \infty$  are associated with the model integrability.

For  $\alpha\nu$  fermion branches with  $N_{\alpha\nu} > 0$  finite occupancy in a given state the maximum  $\nu$  value  $\nu_{max}$  obeys the inequality  $\nu_{max} \leq C_\alpha$ . The absolute maximum value  $\nu_{max} = C_\alpha$  is reached for a subspace with one  $\alpha\nu$  fermion and vanishing occupancies for the remaining  $\alpha\nu'$  branches such that  $\nu' \neq \nu$ . For the states spanning such a subspace the  $2C_\alpha$   $\eta$ -spinons ( $\alpha = \eta$ ) or spinons ( $\alpha = s$ ) other than the independent  $\eta$ -spinons or independent spinons, respectively, are part of a single  $\alpha\nu$  fermion, which moves around in a  $\alpha\nu$  effective lattice with  $2S_\alpha$  unoccupied sites. For  $S_\alpha = 0$  such a single  $\alpha\nu$  bond particle has a "Big-Bang" like character in that the  $\eta$ -spin ( $\alpha = \eta$ ) or spin ( $\alpha = s$ ) degrees of freedom of a half-filling  $N = N_a^D$  state with an equal number  $N_a^D/2 = \nu_{max}$  of doubly and unoccupied sites or  $N_a^D = 2\nu_{max}$  sites singly occupied by an equal number  $N_a^D/2 = \nu_{max}$  of spin-up and spin-down electrons, respectively, are described by such an object. Such two Big-Bang states have  $\eta$ -spin and spin lattice site numbers: (i)  $N_{a_\eta}^D = 2\nu_{max} = N_a^D$  and  $N_{a_s}^D = 0$  referring to a single  $\eta$ -spin-neutral  $\nu = N_a^D/2$  and  $N_a^D$ - $\eta$ -spinon composite  $\eta\nu$  fermion in a  $\eta\nu$  band lattice with a single vanishing momentum value and an empty  $c$  momentum band with  $N_c^h = N_a^D$   $c$  fermion holes; (ii)  $N_{a_\eta}^D = 0$  and  $N_{a_s}^D = 2\nu_{max} = N_a^D$  corresponding to a single spin-neutral  $\nu = N_a^D/2$  and  $N_a^D$ -spinon composite  $s\nu$  fermion in a  $s\nu$  band with a single vanishing momentum value and a full  $c$  momentum band filled by  $N_c = N_a^D$   $c$  fermions. It turns out that such Big Bang  $\alpha\nu$  fermions are invariant under the electron - rotated-electron unitary transformation. That invariance implies that they are  $N$ -electron objects and hence the corresponding Big-Bang states have vanishing overlap with one- and two-electron excitations: Their creation requires application onto the ground state whose occupancy configurations we study below of a suitable  $N$ -electron operator. As a result in part of their invariance under the electron - rotated-electron unitary transformation, the  $N$ -electron excited state generated by creation of such objects is an exact energy eigenstate both for the model on the 1D and square lattice.

## B. Processes that conserve and do not conserve the number of sites of the $\eta$ -spin and spin effective lattices

The vacuum (23) of the theory corresponds to  $N_{a_\eta}^D$  independent  $+1/2$   $\eta$ -spinons and  $N_{a_s}^D$  independent  $+1/2$  spinons so that as mentioned above such objects play the role of "unoccupied sites" of the  $\eta$ -spin and spin effective lattices, respectively. Consistently, the latter objects have vanishing energy and momentum and relative to that vacuum their  $\eta$ -spin and spin flip processes correspond to "creation" processes of independent  $-1/2$   $\eta$ -spinons and independent  $-1/2$  spinons, respectively.

Furthermore, creation of a local  $\eta\nu$  fermion involves the replacement of  $2\nu$  independent  $+1/2$   $\eta$ -spinons corresponding to  $2\nu$  sites of the  $\eta$ -spin effective lattice by  $\nu - 1/2$   $\eta$ -spinons and  $\nu + 1/2$   $\eta$ -spinons in the  $\eta$ -spin-neutral configuration associated with such a  $\eta\nu$  fermion. Also creation of a local  $s\nu$  fermion involves the replacement of  $2\nu$  independent  $+1/2$  spinons referring to  $2\nu$  sites of the spin effective lattice by  $\nu - 1/2$  spinons and  $\nu + 1/2$  spinons in the spin-neutral configuration associated with such a  $s\nu$  fermion. Finally, creation (and annihilation) of a  $c$  fermion involves annihilation (and creation) of a  $c$  fermion hole. The latter process involves removal (and addition) of one site from (and to) the  $\eta$ -spin effective lattice and addition (and removal) of one site to (and from) the spin effective lattice.

The momentum eigenstates considered in this paper are generated by microscopic momentum occupancy configurations of  $c$  and  $\alpha\nu$  fermions. Such configurations can be expressed as a superposition of local rotated-electron occupancies in the original lattice. The degrees of freedom of the rotated-electron occupancy of a given site of the original lattice are always of two types. For the sites singly occupied by a rotated electron of spin projection  $-1/2$  or  $+1/2$ , those are a spinless  $c$  fermion of charge  $-e$  associated with the  $U(1)$  symmetry and a spinon of spin projection  $-1/2$  or  $+1/2$  associated with the spin  $SU(2)$  symmetry, respectively. In turn, for the sites doubly occupied or unoccupied by rotated electrons, those are a  $\eta$ -spinless  $c$  fermion hole associated with the  $U(1)$  symmetry and a  $\eta$ -spinon of  $\eta$ -spin projection  $-1/2$  or  $+1/2$  associated with the  $\eta$ -spin  $SU(2)$  symmetry, respectively.

It follows that the  $2\nu$  sites of the spin effective lattice occupied by one local  $s\nu$  fermion correspond to the spin degrees of freedom of  $2\nu$  rotated-electron singly occupied sites whose charge degrees of freedom are described by  $2\nu$  occupied sites of the  $c$  fermion lattice. Therefore, these  $2\nu$  rotated-electron singly occupied sites are described both by the local  $s\nu$  fermion and  $2\nu$  local  $c$  fermions.

Moreover, the  $2\nu$  sites of the  $\eta$ -spin effective lattice occupied by one local  $\eta\nu$  fermion correspond to the  $\eta$ -spin degrees of freedom of  $\nu$  rotated-electron doubly occupied sites and  $\nu$  rotated-electron unoccupied sites whose  $U(1)$  symmetry degrees of freedom are described by  $2\nu$  unoccupied sites of the  $c$  fermion lattice. As a result, the  $\nu$  rotated-electron doubly occupied sites and  $\nu$  rotated-electron unoccupied sites are described both by the local  $\eta\nu$  fermion and  $2\nu$  local  $c$  fermion holes ( $c$  effective lattice unoccupied sites).

In summary, local  $s\nu$  fermions share  $2\nu$  sites of the original lattice with  $2\nu$  local  $c$  fermions and local  $\eta\nu$  fermions share  $2\nu$  sites of that lattice with  $2\nu$  local  $c$  fermion holes. Any pair of local  $\alpha\nu$  and  $\alpha'\nu'$  fermions always refer to

two *different* sets of  $2\nu$  and  $2\nu'$  sites, respectively, of the original lattice. Creation of local  $\eta\nu$  and  $s\nu$  fermions are processes that conserve the total number of  $\eta$ -spinons and spinons, respectively, and hence also conserve the number of  $c$  fermions and  $c$  fermion holes. In contrast, creation (and annihilation) of one local  $c$  fermion is a process that involves addition (and removal) of one site to (and from) the spin effective lattice and removal (and addition) of one site from (and to) the  $\eta$ -spin effective lattice. Therefore, the spin and  $\eta$ -spin effective lattices are exotic, since the number of their sites  $N_{a_s}^D = 2S_c$  and  $N_{a_\eta}^D = [N_a^D - 2S_c]$ , respectively, changes by  $\pm 1$  and  $\mp 1$  upon creation/annihilation of one  $c$  fermion. Indeed, such processes change the eigenvalue  $S_c$  of the generator (7) of the global  $U(1)$  symmetry. A subspace with constant  $S_c$  value and hence constant  $N_{a_\eta}^D = [N_a^D - 2S_c]$  and  $N_{a_s}^D = 2S_c$  values as well is associated with a well-defined vacuum  $|0_{\eta s}\rangle$  given in Eq. (23). An excitation involving a change of such values drives the system into a new subspace referring to a different vacuum  $|0_{\eta s}\rangle$ . In turn,  $\eta$ -spinon and spinon creation and annihilation processes refer to excitations within the same quantum-liquid subspace associated with a well-defined vacuum  $|0_{\eta s}\rangle$ .

It follows that from the point of view of the  $\eta$ -spin and spin degrees of freedom,  $c$  fermion creation and annihilation processes correspond to a change of quantum system. Indeed, the  $\eta$ -spin and spin lattices and corresponding number of sites change along with the quantum-system vacuum  $|0_{\eta s}\rangle$  of Eq. (23). Therefore, within the  $\eta$ -spinon and spinon representation there is a different quantum system for each eigenvalue  $S_c$  of the generator (7) of the global  $U(1)$  symmetry. However, from the point of view of the degrees of freedom associated with the latter symmetry, the model (1) corresponds to a single quantum system and the local  $c$  fermions live on a lattice whose number of sites  $N_a^D = [N_{a_s}^D + N_{a_\eta}^D]$  is constant, alike that of the electrons and rotated electrons. Consistently, the  $c$  effective lattice is identical to the original lattice. This property follows from the invariance of the latter lattice under the electron - rotated-electron unitary transformation, which is related to the invariance of the momentum operator of Eq. (5).

Creation of local  $\eta\nu$  (and  $s\nu$ ) fermions always involves virtual processes where  $2\nu$  independent  $+1/2$   $\eta$ -spinons (and  $2\nu$  independent  $+1/2$  spinons) are replaced by the  $\eta$ -spin-singlet (and spin-singlet)  $2\nu$ -site occupancy configurations of the local  $\eta\nu$  fermions (and  $s\nu$  fermions) in the  $\eta$ -spin (and spin) effective lattice. For instance, a given process for which two local  $s1$  fermions of the initial state are replaced by one local  $s2$  fermion in the final state is divided into two virtual processes: first, two local  $s1$  fermions are annihilated, *i.e.* the four sites of the spin effective lattice occupied in the initial state by the local  $s1$  fermions are upon two spin-flip processes occupied in an intermediate virtual state by four independent  $+1/2$  spinons (annihilation of two  $s1$  bond particles); second, one local  $s2$  fermion is created on such four sites. That involves two opposite spin-flip processes and rearrangement of the spinons associated with the creation of the local  $s2$  fermion spin-neutral four-spinon occupancy configurations in the spin effective lattice.

Concerning creation (and annihilation) of one local  $c$  fermion, the corresponding overall excitation always involves a virtual process for which the site of the  $\eta$ -spin effective lattice removed (and added) by such an elementary process is occupied in the initial (and final) state by an independent  $+1/2$   $\eta$ -spinon. Also the site of the spin effective lattice added (and removed) by such an elementary process is occupied in the final (and initial) state by an independent  $+1/2$  spinon.

If as occurs for one-electron addition (and removal), creation (and annihilation) of a local  $c$  fermion involves creation (and annihilation) of a local  $s1$  fermion, the overall process is divided into two virtual processes. For instance, complementarily to creation of the local  $c$  fermion in its effective lattice, the virtual processes occurring in the spin effective lattice are: First, a site occupied by an independent  $+1/2$  spinon is added to that lattice; Second, a local  $s1$  fermion is created, one of the two independent  $+1/2$  spinons involved in the final-state two-site  $s1$  bond configuration being that located on the site added to the spin effective lattice. (A corresponding momentum eigenstate involves the superposition of many local configurations for which that site has different positions.) In turn, if annihilation of a local  $c$  fermion at its effective lattice involves annihilation of a local  $s1$  fermion, one has the following virtual processes in the spin effective lattice: First, a local  $s1$  fermion is annihilated, what involves a rearrangement process, which leads to the occupancy of its two sites by two independent  $+1/2$  spinons in the intermediate virtual state; Second, the site of the spin effective lattice occupied by one of these two independent spinons is removed along with it.

Creation (and annihilation) of both one local  $c$  fermion and one local  $s1$  fermion corresponds to creation (and annihilation) of a spin-down electron. In turn, the corresponding process of creation (and annihilation) of a spin-up electron involves addition (and removal) of one local  $c$  fermion to (and from) its effective lattice and addition (and removal) of one site occupied by an independent  $+1/2$  spinon to (and from) the spin effective lattice. Alike creation and annihilation of local  $c$  fermions leads to addition and removal (and removal and addition) of sites in the spin (and  $\eta$ -spin) effective lattice, respectively, it is confirmed below that creation of one local  $\alpha\nu'$  fermion gives rise to addition of  $2\nu'$  sites to the  $\alpha\nu$  effective lattices of  $\alpha\nu$  fermion branches such that  $\nu < \nu'$ .

It is confirmed below in Section V that for the states that span the one- and two-electron subspace only  $c$  fermions and  $s1$  fermions play an active role. Concerning excitations belonging to such a subspace that conserve the number  $N_c = 2S_c$  of  $c$  fermions and thus the eigenvalues  $S_c$  of the generator (7) of the global  $U(1)$  symmetry and the number  $N_{s1}$  of  $s1$  fermions, the  $c$  fermions can move through their effective lattice independently of the motion of the corresponding  $s1$  fermions. In that case when a given  $c$  fermion moves around in the lattice it is not attached always to the same spinon and hence to the same two-spinon  $s1$  fermion. The investigations of Ref.<sup>22</sup> reveal that there are

correlations between a spin-neutral two-spinon  $s1$  fermion and a well defined set of  $c$  fermion pairs whose centre of mass is located at the  $s1$  fermion position.

### C. Ranges of the $\alpha\nu$ fermion and $c$ fermion energies, transformation laws of such objects, and the ground-state occupancies

The quantum-object occupancy configurations of the ground state are found below. Self-consistency of our description then confirms that for  $m \geq 0$  and  $x \geq 0$  the elementary energies  $\epsilon_{s,-1/2} = 2\mu_B H$  and  $\epsilon_{\eta,-1/2} = 2\mu$  of Eq. (A7) of Appendix A correspond to creation onto the ground state of an independent  $-1/2$  spinon and an independent  $-1/2$   $\eta$ -spinon, respectively. We recall that  $\mu_B$  is the Bohr magneton and  $H$  the magnitude of a magnetic field aligned parallel to the plane (2D) or chain (1D). The energy  $\epsilon_{s,-1/2} = 2\mu_B H$  (and  $\epsilon_{\eta,-1/2} = 2\mu$ ) refers to an elementary spin-flip (and  $\eta$ -spin-flip) process, which transforms an independent  $+1/2$  spinon (and  $+1/2$   $\eta$ -spinon) into an independent  $-1/2$  spinon (and  $-1/2$   $\eta$ -spinon). Such elementary energies control the range of several physically important energy scales. Since within our LWS representation an independent  $+1/2$  spinon (and  $+1/2$   $\eta$ -spinon) has vanishing energy and an independent  $-1/2$  spinon (and  $-1/2$   $\eta$ -spinon) has an energy given by  $\epsilon_{s,-1/2} = 2\mu_B H$  (and  $\epsilon_{\eta,-1/2} = 2\mu$ ), the energy of a pair of independent spinons (and  $\eta$ -spinons) with opposite projections is  $2\mu_B H$  (and  $2\mu$ ). Indeed, due to the invariance of such objects under the electron - rotated-electron unitary transformation, they are not energy entangled and the total energy is the sum of their individual energies.

The magnetization curve is such that the spin density  $m$  vanishes at  $H = 0$  and is finite and positive for  $H > 0$ . (We recall that within the LWS representation the convention that  $\mu > 0$  for  $x > 0$  and  $H > 0$  for  $m > 0$  is used.) Consistently with the properties of the  $x = 0$  and  $m = 0$  absolute ground state discussed below and in Ref.<sup>1</sup>, for  $x = 0$  and  $m = 0$  the chemical potential  $\mu$  belongs to the range  $\mu \in (-\mu^0, \mu^0)$  where the energy scale  $\mu^0 \equiv \lim_{x \rightarrow 0} \mu$  equals one half the Mott-Hubbard gap and is such that  $\mu^0 \rightarrow 0$  for  $U/4t \rightarrow 0$  and  $\mu^0 > 0$  for  $U/4t > 0$ . For  $0 < x < 1$  and  $m = 0$  the chemical potential is an increasing function of the hole concentration  $x$  such that,

$$\mu^0 \leq \mu(x) \leq \mu^1; \quad 0 < x < 1, \quad m = 0, \quad (32)$$

where  $\mu^1 \equiv \lim_{x \rightarrow 1} \mu$ .  $\mu^1$  reads,

$$\mu^1 = U/2 + 2Dt; \quad D = 1, 2. \quad (33)$$

In turn,  $\mu^0$  has the following limiting behaviors,

$$\mu^0 \approx \frac{U}{2\pi^2} \left( \frac{[8\pi]^2 t}{U} \right)^{D/2} e^{-2\pi(\frac{1}{t})^{1/D}}, \quad U/4t \ll 1; \quad \mu^0 \approx [U/2 - 2Dt], \quad U/4t \gg 1, \quad D = 1, 2. \quad (34)$$

Hence indeed  $\mu^0 \rightarrow 0$  as  $U/4t \rightarrow 0$  whereas  $\mu^0 \rightarrow \infty$  for  $U/4t \rightarrow \infty$  for both the model on the 1D and square lattices.

For  $D = 1$  the expressions provided in Eq. (32)-(34) are obtained by use of the exact Bethe-ansatz solution<sup>15</sup>. Expression (33) is exact both for 1D and the square lattice. It can be derived explicitly for both lattices, since it refers to the non-interacting limit of vanishing electronic density. In turn, the expressions given in Eq. (34) for the model on the square lattice are obtained by the use of a result discussed in Subsection VI-A: the energy below which the long-range antiferromagnetic order survives for  $x = 0$ ,  $m = 0$ , and zero temperature is  $\mu^0$  where  $2\mu_0$  is the Mott-Hubbard gap. Indeed, according to the analysis of that subsection the Mott-Hubbard gap  $2\mu^0$ , which refers to the charge degrees of freedom, affects the spin degrees of freedom as well. Consistently, the  $D = 2$  limiting behaviors  $\mu^0 \approx 32te^{-2\pi\sqrt{t/U}}$  and  $\mu^0 \approx U/2$  of Eq. (34) for  $U/4t \ll 1$  and  $U/4t \gg 1$ , respectively, are those of the zero-temperature spin gap of Eq. (13) of Ref.<sup>29</sup>.

In the following we confirm that ground states have no  $\eta\nu$  fermions and no  $s\nu$  fermions with  $\nu \geq 2$  spinon pairs. Hence the corresponding energies  $\epsilon_{\eta\nu}$  and  $\epsilon_{s\nu}$ , respectively, considered below refer to creation onto the ground state of one of such objects carrying a given momentum. We start by providing a set of useful properties. We emphasize that some of these properties are not valid for descriptions generated by rotated-electron operators associated with the general unitary operators  $\hat{V}$  considered in Ref.<sup>2</sup>. Indeed, the following properties refer to the operator description associated with the rotated-electron operators  $\tilde{c}_{\vec{r}_j, \sigma}^\dagger = \hat{V}^\dagger c_{\vec{r}_j, \sigma}^\dagger \hat{V}$  of Eq. (8) as defined in this paper, whose electron - rotated-electron unitary operator  $\hat{V} = \hat{V}(U/4t)$  is such that the set of  $4^{N_a^D}$  states of the form  $|\Psi_{U/4t}\rangle = \hat{V}^\dagger |\Psi_\infty\rangle$  are energy eigenstates for  $U/4t > 0$ . Here  $|\Psi_\infty\rangle$  corresponds to exactly one of the many set of  $U/4t \rightarrow \infty$  energy eigenstates, chosen according to the well-defined criterion discussed above in Subection II-A. For the model on the square lattice our operator description refer to a related complete set of  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates  $|\Phi_{U/4t}\rangle = \hat{V}^\dagger |\Phi_\infty\rangle$  generated from the corresponding  $U/4t \rightarrow \infty$  states  $|\Phi_\infty\rangle$  by the same electron - rotated-electron

unitary operator  $\hat{V} = \hat{V}(U/4t)$  as the energy eigenstates  $|\Psi_{U/4t}\rangle = \hat{V}^\dagger |\Psi_\infty\rangle$ . Some of the states  $|\Phi_{U/4t}\rangle$  are identical to the energy eigenstates  $|\Psi_{U/4t}\rangle$ , which are also  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates. (For the 1D model both sets of states are identical for the whole Hilbert space.)

Let us profit from the interplay of the transformation laws of the  $\alpha\nu$  fermions under the electron - rotated-electron unitary transformation with the model global  $SO(3) \times SO(3) \times U(1)$  symmetry to reach valuable information about the range of the energy  $\epsilon_{\alpha\nu}$  for addition onto the ground state of one  $\alpha\nu$  fermion. For the model on the square lattice there is in general a small uncertainty  $\delta\epsilon$  in the energy  $\epsilon_{\alpha\nu}$  of a  $\alpha\nu$  fermion of a given momentum smaller than or equal to the corresponding energy bandwidth and such that  $\epsilon_{\alpha\nu} \pm \delta\epsilon$  belongs to that energy range. For that model and  $\alpha\nu$  fermions that are invariant under the electron - rotated-electron unitary transformation one has  $\delta\epsilon = 0$ . That holds for instance for the  $\alpha\nu$  fermions whose occupancy configurations generate above states  $|\Phi_{U/4t}\rangle$  that are identical to energy eigenstates  $|\Psi_{U/4t}\rangle$ . For both the model on the 1D and square lattices the latter range corresponds to the energy bandwidth of the energy dispersion  $\epsilon_{\alpha\nu}$ . For the description associated with rotated-electrons, corresponding  $c$  fermions,  $\eta$ -spinons, and spinons whose operators are given in Eqs. (8)-(17), and composite  $\eta$ -spinon and spinon fermions the following properties hold.

### 1. Energy range of a $\eta\nu$ fermion

A  $\eta\nu$  fermion is a  $\eta$ -spin-neutral anti-bounding configuration of  $\nu - 1/2$   $\eta$ -spinons and  $\nu + 1/2$   $\eta$ -spinons. Symmetry implies that for  $U/4t > 0$  there is no energy overlap between the ranges of bandwidth  $W_{\eta\nu}$  of the energy  $\epsilon_{\eta\nu}$  corresponding to different branches  $\nu = 1, \dots, C_\eta$  associated with addition onto the ground state of one  $\eta\nu$  fermion of a given momentum. Since fermions belonging to neighboring branches  $\eta\nu$  and  $\eta\nu + 1$  differ in the number of single  $\eta$ -spinon pairs by one, the requirement for the above lack of energy overlap is that  $W_{\eta\nu} \leq 2\mu$  where  $2\mu$  equals the energy of a pair of independent  $\eta$ -spinons of opposite  $\eta$ -spin projections. Such properties imply that the energy  $\epsilon_{\eta\nu}$  obeys the following inequality,

$$2\nu\mu \leq \epsilon_{\eta\nu} < 2(\nu + i_{\eta\nu})\mu; \quad 0 \leq i_{\eta\nu} \leq 1, \quad (35)$$

where  $2\nu\mu$  is the energy for creation of  $\nu - 1/2$  independent  $\eta$ -spinons and  $\nu$  independent  $+1/2$   $\eta$ -spinons onto the ground state. Since the latter objects are invariant under the electron - rotated-electron unitary transformation associated with the operator  $\hat{V}$ , they are non interacting and thus their energies are additive. For  $m = 0$  the number  $i_{\eta\nu}$  decreases continuously for increasing values of  $U/4t$ , having the limiting behaviors  $i_{\eta\nu} \rightarrow 1$  for  $U/4t \rightarrow 0$  and  $i_{\eta\nu} \rightarrow 0$  for  $U/4t \rightarrow \infty$  so that  $W_{\eta\nu} \rightarrow 0$  as  $U/4t \rightarrow \infty$ . The latter behavior is associated with the full degeneracy of the  $\eta$ -spin configurations reached for  $U/4t \rightarrow \infty$  when the spectrum of the  $2\nu$ - $\eta$ -spinon composite  $\eta\nu$  fermion becomes dispersionless.

### 2. Energy range of a $s\nu$ fermion

A  $s\nu$  fermion of a given momentum is a spin-neutral bounding configuration of  $\nu - 1/2$  spinons and  $\nu + 1/2$  spinons. Again, symmetry implies that for  $U/4t > 0$  there is no energy overlap between the ranges of bandwidth  $W_{s\nu}$  of the one- $s\nu$  fermion energy  $\epsilon_{s\nu}$  associated with different branches  $\nu = 1, \dots, C_s$ . For  $s\nu$  branches with a number of spinon pairs  $\nu \geq 2$  the bandwidth  $W_{s\nu}$  of such an energy range is for the present bounding configurations and for the same reasoning as for the  $\eta\nu$  fermion such that  $W_{s\nu} \leq 2\mu_B H$  where  $2\mu_B H$  equals the energy of a pair of independent spinons of opposite spin projections. The energy  $\epsilon_{s\nu}$  for addition onto the ground state of one  $s\nu$  fermion with  $\nu \geq 2$  spinon pairs obeys the inequality,

$$2(\nu - i_{s\nu})\mu_B H \leq \epsilon_{s\nu} \leq 2\nu\mu_B H; \quad \nu > 1, \quad 0 \leq i_{s\nu} \leq 1, \quad (36)$$

where  $2\nu\mu_B H$  is the energy for creation of  $\nu$  independent  $-1/2$  spinons and  $\nu$  independent  $+1/2$  spinons onto the ground state. Since the latter objects are invariant under the unitary transformation associated with the operator  $\hat{V}$ , they are not energy entangled and their energies are additive. For  $m = 0$  the number  $i_{s\nu}$  decreases continuously for increasing values of  $U/4t$ , having the limiting behaviors  $i_{s\nu} \rightarrow 1$  for  $U/4t \rightarrow 0$  and  $i_{s\nu} \rightarrow 0$  for  $U/4t \rightarrow \infty$  so that  $W_{s\nu} \rightarrow 0$  as  $U/4t \rightarrow \infty$ . Such a behavior is associated with the full degeneracy of the spin configurations reached for  $U/4t \rightarrow \infty$  when the spectrum of the  $2\nu$ -spinon composite  $s\nu$  fermion becomes dispersionless.

In turn, for a  $m = 0$  and  $x \geq 0$  ground state all sites of the  $s1$  effective lattice are occupied so that the corresponding  $s1$  momentum band is full and the energy  $-\epsilon_{s1}$  for removal from that state of one  $s1$  fermion carrying momentum obeys the inequality,

$$0 \leq -\epsilon_{s1} \leq \max \{W_{s1}, |\Delta|\}, \quad (37)$$

where the energy scale  $|\Delta|$  is introduced below in Subsection VI-B and further studied in Ref.<sup>1</sup>. For small hole concentrations  $0 < x \ll 1$  it vanishes both in the limits  $U/4t \rightarrow 0$  and  $U/4t \rightarrow \infty$  and goes through a maximum value at  $U/4t = u_0 \approx 1.302$  and at constant  $U/4t$  decreases for increasing  $x$  and vanishes for  $x > x_*$  where the critical hole concentration  $x_*$  is studied in Ref.<sup>1</sup> for approximately  $U/4t \geq u_0$ . As discussed in that subsection, due to a sharp quantum phase transition it has a singular behavior at  $x = 0$ , having for  $U/4t > 0$  different magnitudes at  $x = 0$  and  $x \rightarrow 0$ , respectively. In turn, for  $m = 0$  the energy bandwidth  $W_{s1}$  refers to the auxiliary  $s1$  fermion dispersion defined in Ref.<sup>1</sup> and has its maximum magnitude at  $U/4t = 0$ . For  $U/4t > 0$  it decreases monotonously for increasing values of  $U/4t$ , vanishing for  $U/4t \rightarrow \infty$ . That both  $W_{s1} \rightarrow 0$  and  $|\Delta| \rightarrow 0$  for  $U/4t \rightarrow \infty$  is associated with the full degeneracy of the spin configurations reached in that limit for which the spectrum of the two-spinon composite  $s1$  fermions becomes dispersionless. For instance, we could access the explicit limiting behaviors of the  $m = 0$  energy bandwidth  $W_{s1}^0 \equiv \lim_{x \rightarrow 0} W_{s1} = W_{s1}|_{x=0}$ ,

$$W_{s1}^0 = 2Dt, \quad U/4t = 0; \quad W_{s1}^0 \approx 2D\pi \frac{t^2}{U}, \quad U/4t \gg 19^{D-1}, \quad D = 1, 2, \quad (38)$$

where that for the  $D = 2$  square lattice the large- $U/4t$  expression is valid for  $U/4t \gg 19$  is justified below in Section VI.

In the  $U/4t \rightarrow \infty$  limit the  $s1$  fermion occupancy configurations that generate the spin degrees of freedom of spin-density  $m = 0$  ground states considered below become for the 1D model those of the spins of the spin-charge factorized wave function introduced both by Woynarovich<sup>42</sup> and Ogata and Shiba<sup>43</sup>. In turn, for the model on the square lattice such configurations become in that limit and within a mean-field approximation for the fictitious magnetic field  $\vec{B}_{s1}$  of Eq. (25) those of a full lowest Landau level with  $N_{s1} = N_{a_{s1}}^2 = N/2$  one- $s1$ -fermion degenerate states of the 2D quantum Hall effect<sup>1</sup>. Here  $N_{a_{s1}}^2$  is the number of both sites of the square  $s1$  effective lattice and  $s1$  band discrete momentum values. For finite  $U/4t$  values and  $x > 0$  the degeneracy of the  $N_{a_{s1}}^2 = N/2$  one- $s1$  fermion states of the square-lattice quantum liquid is removed by the emergence of a finite-energy-bandwidth  $s1$  fermion dispersion yet the number of  $s1$  band discrete momentum values remains being given by  $N_{a_{s1}}^2 = B_{s1} L^2 / \Phi_0$  and the  $s1$  effective lattice spacing by  $a_{s1} = l_{s1} / \sqrt{2\pi}$  where  $l_{s1}$  is the fictitious-magnetic-field length and we recall that in our units the fictitious-magnetic-field flux quantum reads  $\Phi_0 = 1$ <sup>1</sup>.

### 3. The energy range of the $c$ fermions

The energy  $\epsilon_c$  for addition onto the ground state of one  $c$  fermion of a given momentum and the energy  $-\epsilon_c$  for removal from that state such a  $c$  fermion obey the inequalities,

$$0 \leq \epsilon_c \leq W_c^h = [4Dt - W_c^p]; \quad 0 \leq -\epsilon_c \leq W_c^p, \quad D = 1, 2, \quad (39)$$

respectively. Here  $W_c^h = [4Dt - W_c^p] \in (0, 4Dt)$  increases monotonously for increasing values of hole concentration  $x \in (0, 1)$ . The energy bandwidth  $W_c^p$  depends little on  $U/4t$  and for  $U/4t > 0$  has the following limiting behaviors,

$$W_c^p = 4Dt, \quad x = 0; \quad W_c^p = 0; \quad x = 1. \quad (40)$$

### 4. Transformation laws of $\alpha\nu$ fermions and $c$ fermions under the electron - rotated-electron unitary transformation

An useful property is that  $\eta\nu$  fermions and  $s\nu$  fermions with  $\nu \geq 2$  spinon pairs that remain invariant under the electron - rotated-electron unitary transformation have energy given by,

$$\epsilon_{\eta\nu} = 2\nu\mu, \quad \nu = 1, \dots, C_\eta; \quad \epsilon_{s\nu} = 2\nu\mu_B H, \quad \nu = 2, \dots, C_s. \quad (41)$$

Those are non-interacting objects such that their energy is additive in the individual energies of the corresponding  $2\nu$   $\eta$ -spinons and spinons, respectively. Therefore, for  $U/4t > 0$  they refer to the same occupancy configurations in terms of both rotated electrons and electrons. However, note that in contrast to the independent  $\eta$ -spinons or independent spinons here the objects that are invariant under the electron - rotated-electron unitary transformation are the composite  $2\nu$ - $\eta$ -spinon  $\eta\nu$  fermions or  $2\nu$ -spinon  $s\nu$  fermions and not the corresponding individual  $2\nu$   $\eta$ -spinons or  $2\nu$ -spinons, respectively. In turn,  $\eta\nu$  fermions and  $s\nu$  fermions with  $\nu \geq 2$  spinon pairs whose energies obey the inequalities  $\epsilon_{\eta\nu} > 2\nu\mu$  and  $\epsilon_{s\nu} < 2\nu\mu_B H$  are not invariant under the electron - rotated-electron transformation. Furthermore, for finite  $U/4t$  values  $c$  fermions and  $s1$  fermions are not invariant under that transformation.

Both for the model on the 1D and square lattices the initial ground state and the excited states generated by creation of one  $\eta\nu$  fermion or  $s\nu$  fermion whose energy is given by (41) are energy eigenstates.

### 5. Ground state occupancies

Fulfillment of the requirement of self-consistency concerning the set of properties given here, reveals that both for the model on the 1D and square lattices the subspace spanned by the  $x > 0$  and  $m > 0$  LWS ground states and their excited energy eigenstates of energy  $\omega < \min\{2\mu, 2\mu_B H\}$  there are no  $-1/2$   $\eta$ -spinons,  $\eta\nu$  fermions, independent  $-1/2$  spinons, and  $s\nu'$  fermions with  $\nu' \geq 2$  spinon pairs so that  $N_{\eta\nu} = 0$  and  $N_{s\nu'} = 0$  for  $\nu' \geq 2$ . Hence the number of  $c$  fermions is  $N_c = 2S_c = N = (1-x)N_a^D$ , independent  $+1/2$   $\eta$ -spinons  $L_{\eta,+1/2} = 2S_\eta = [N_a^D - N] = xN_a^D$ , independent  $+1/2$  spinons  $L_{s,+1/2} = 2S_s = [N_\uparrow - N_\downarrow] = mN_a^D$ , and  $s1$  fermions  $N_{s1} = N_\downarrow$ .

From analysis and comparison of the occupancies of the spin LWS ground states ( $m > 0$ ) and spin highest-weight state (HWS) ground states ( $m < 0$ ), one finds that a  $m = 0$  ground state for which  $N$  is even and  $x \geq 0$  has no  $-1/2$   $\eta$ -spinons,  $\eta\nu$  fermions, independent  $\pm 1/2$  spinons, and  $s\nu'$  fermions with  $\nu' > 1$  spinon pairs so that  $N_{\eta\nu} = 0$  and  $N_{s\nu'} = 0$  for  $\nu' > 1$ . Hence the number of  $c$  fermions is  $N_c = 2S_c = N = (1-x)N_a^D$ , independent  $+1/2$   $\eta$ -spinons  $L_{\eta,+1/2} = 2S_\eta = [N_a^D - N] = xN_a^D$ , and  $s1$  fermions  $N_{s1} = N/2 = (1-x)N_a^D/2$ .

#### D. The number of sites of the $\alpha\nu$ effective lattices and discrete momentum values of the $\alpha\nu$ bands

A local  $\eta\nu$  (and  $s\nu$ ) fermion refers to a superposition of well-defined  $\eta$ -spinon (and spinon) occupancy configurations involving  $2\nu$  sites of the  $\eta$ -spin (and spin) effective lattice. The number of sites of the  $s1$  effective lattice plays an important role in the study of the model in the one- and two-electron subspace considered below in Subsection V-A. In order to evaluate its expression one needs to solve the same problem for the remaining  $\alpha\nu$  effective lattices as well. Indeed, the values of the set of numbers  $\{N_{a\alpha\nu}^D\}$  are dependent of each other. Fortunately, in the limit  $N_a^D \gg 1$  one does not need detailed information about the occupancy configurations of the  $\eta$ -spin (and spin) effective lattice whose superposition defines the internal structure of a  $\eta\nu$  (and  $s\nu$ ) fermion to achieve such a goal. The only needed information is that the  $2\nu$  sites of the  $\eta$ -spin (or spin) effective lattice involved in such configurations are centered at a point of real-space coordinate  $\vec{r}_j$ , which defines the real-space coordinate of the local  $\alpha\nu$  fermion. Here  $j = 1, \dots, N_{a\alpha\nu}^D$  of a given subspace where  $N_{a\alpha\nu}^D$  is the number of sites of the  $\alpha\nu$  effective lattice. Our goal is the derivation of the expression for that number in terms of the set of numbers  $N_c$  and  $\{N_{\alpha'\nu'}\}$  where  $\alpha' = \eta, s$  and  $\nu' = 1, 2, 3, \dots, C_{\alpha'\nu'}$ . The real-space coordinate  $\vec{r}_j$  plays the role of "centre of mass" of the local  $\alpha\nu$  fermion and has  $N_{a\alpha\nu}^D$  well-defined values associated with the sites of the  $\alpha\nu$  effective lattice.

For  $N_a^D \gg 1$  (i) the internal structure of a local  $\alpha\nu$  fermion and (ii) its real-space position  $\vec{r}_j$  are separated problems. The present analysis refers to the problem (ii) only. The problem (i) is addressed for the  $s1$  bond particle associated with the local  $s1$  fermion in Ref.<sup>18</sup>. Concerning the internal structure of a local  $\alpha\nu$  fermion, the only issue that matters for the present analysis is that the  $2\nu$  sites of the  $\eta$ -spin (and spin) effective lattice occupied by a given local  $\eta\nu$  (and  $s\nu$ ) fermion correspond to  $2\nu$  sites of the original lattice that are not simultaneously occupied by any other such fermions.

The number of sites  $N_{a\alpha\nu}^D$  of the  $\alpha\nu$  effective lattice is an integer number. We emphasize, however, that for the model on the square lattice for which  $D = 2$  the related number  $N_{a\alpha\nu}$  is not in general integer so that the  $\alpha\nu$  effective lattice is not a perfect square. However, for  $N_{a\alpha\nu}/N_a$  finite and  $N_a^2 \gg 1$  it is nearly a square lattice so that in that limit we use the notation  $N_{a\alpha\nu}^2$  for its number of sites.

The  $\alpha\nu$  effective lattice and its  $N_{a\alpha\nu}^D$  sites are well-defined concepts in a subspace for which the values of the set of numbers  $N_c = 2S_c$  and  $\{N_{\alpha'\nu'}\}$  where  $\nu' = 1, 2, 3, \dots, C_\alpha$  remain constant. As justified below, this is equivalent to the  $\eta$ -spin  $S_\eta$  ( $\alpha = \eta$ ) or spin  $S_s$  ( $\alpha = s$ ) and values of the set of numbers  $\{N_{\alpha\nu'}\}$  where  $\nu' = \nu, \nu + 1, \dots, C_\alpha$  remaining constant. For such subspaces the motion of the  $\alpha\nu$  fermion through its effective lattice corresponds to a set of elementary steps where it hops from a given site of well-defined real-space coordinate to another. For the model on the square lattice such elementary steps involve horizontal and vertical virtual steps<sup>18</sup>.

For a local  $\alpha\nu$  fermion the  $2\nu N_{\alpha\nu}$  sites of the  $\eta$ -spin ( $\alpha = \eta$ ) or spin ( $\alpha = s$ ) effective lattice occupied by the  $N_{\alpha\nu}$  local fermions belonging to the same  $\alpha\nu$  branch play the role of the  $N_{\alpha\nu}$  occupied sites of the  $\alpha\nu$  effective lattice. In turn, the  $2S_\eta$  (and  $2S_s$ ) sites of the  $\eta$ -spin (and spin) effective lattice occupied by independent  $+1/2$   $\eta$ -spinons (and spinons) and  $2(\nu' - \nu)$  sites out of the  $2\nu'$  sites of that lattice occupied by each local  $\eta\nu'$  (and  $s\nu'$ ) fermion such that  $\nu' > \nu$  play the role of unoccupied sites of the  $\eta\nu$  (and  $s\nu$ ) effective lattice.

The number of sites of the  $\alpha\nu$  effective lattice is then given by,

$$N_{a\alpha\nu}^D = [N_{\alpha\nu} + N_{\alpha\nu}^h], \quad (42)$$

where the number of unoccupied sites reads,

$$N_{\alpha\nu}^h = [2S_\alpha + 2 \sum_{\nu'=\nu+1}^{C_\alpha} (\nu' - \nu) N_{\alpha\nu'}] = [N_{a_\alpha}^D - \sum_{\nu'=1}^{C_\alpha} (\nu + \nu' - |\nu - \nu'|) N_{\alpha\nu'}]. \quad (43)$$

The equivalence of the two expressions given here confirms that the numbers  $N_c = 2S_c$  and  $\{N_{\alpha\nu'}\}$  where  $\nu' = 1, 2, 3, \dots, C_\alpha$  remaining constant is equivalent to the  $\eta$ -spin  $S_\eta$  ( $\alpha = \eta$ ) or spin  $S_s$  ( $\alpha = s$ ) and values of the set of numbers  $\{N_{\alpha\nu'}\}$  where  $\nu' = \nu, \nu + 1, \dots, C_\alpha$  remaining constant as well. In both cases that implies that  $N_{a_\alpha}^D$  remains constant.

In the following and in Appendix C it is confirmed that the expressions given in Eqs. (42) and (43), which equal the  $\alpha\nu$  band corresponding numbers of discrete momentum values, are compatible with the number of representations of the group  $SO(3) \times SO(3) \times U(1)$  in each subspace with constant values of  $S_c$ ,  $S_\eta$ , and  $S_s$ . From the use of these equations one finds that the number of unoccupied sites of the  $\alpha 1$  effective lattices reads,

$$N_{\alpha 1}^h = [N_{a_\alpha}^D - 2B_\alpha]; \quad B_\alpha = \sum_{\nu=1}^{C_\alpha} N_{\alpha\nu}; \quad \alpha = \eta, s. \quad (44)$$

This number equals that of  $\alpha 1$  fermion holes in the  $\alpha 1$  band.

Straightforward manipulations of the above equations lead to the following general expressions for  $S_\eta$ ,  $S_s$ , and  $S_c$ ,

$$S_\alpha = [\frac{1}{2}N_{\alpha 1}^h - C_\alpha + B_\alpha], \quad \alpha = \eta, s; \quad S_c = [\frac{N_a^D}{2} - \frac{1}{2}N_{\eta 1}^h - B_\eta = \frac{1}{2}N_{s 1}^h + B_s]. \quad (45)$$

It follows from the equality of the two  $S_c$  expressions given Eq. (45) that,

$$\sum_{\alpha=\eta,s} \frac{1}{2}N_{\alpha 1}^h = [\frac{N_a^D}{2} - \sum_{\alpha=\eta,s} B_\alpha]. \quad (46)$$

Equation (31), the first expression of Eq. (45), and Eq. (46) are equivalent to the following sum-rules for the numbers of  $\alpha\nu$  fermions,

$$C_\alpha = \sum_{\nu=1}^{C_\alpha} \nu N_{\alpha\nu} = \frac{1}{2}[N_{a_\alpha}^D - 2S_\alpha]; \quad B_\alpha = \sum_{\nu=1}^{C_\alpha} N_{\alpha\nu} = \frac{1}{2}[N_{a_\alpha}^D - N_{\alpha 1}^h], \quad \alpha = \eta, s, \quad (47)$$

respectively, consistently with the expressions  $C_s = [S_c - S_s]$  and  $C_\eta = [N_a^D - S_c - S_\eta]$  given in Eq. (21).

Each subspace with constant values of  $S_c$  and hence also with constant values of  $N_{a_\eta}^D = [N_a^D - 2S_c]$  and  $N_{a_s}^D = 2S_c$  that the vacuum of the theory given in Eq. (23) refers to can be divided into smaller subspaces with constant values of  $S_c$ ,  $S_\eta$ , and  $S_s$  and hence also with constant values of  $C_\eta$  and  $C_s$ . Furthermore, the latter subspaces can be further divided into even smaller subspaces with constant values for the set of numbers  $\{N_{\eta\nu}\}$  and  $\{N_{s\nu}\}$ , which must obey the sum-rules of Eq. (31).

Let us confirm that expressions (42) and (43) for the number of discrete momentum values of the  $\alpha\nu$  band and  $\alpha\nu$  fermion holes in that band, respectively, are compatible with the number of state representations of the  $U(1)$ ,  $\eta$ -spin  $SU(2)$  ( $\alpha = \eta$ ), and spin  $SU(2)$  ( $\alpha = s$ ) symmetries of the model global  $SO(3) \times SO(3) \times U(1) = [SU(2) \times SU(2) \times U(1)]/Z_2^2$  symmetry in the subspaces with constant values of  $S_c$ ,  $S_\eta$ , and  $S_s$ . Those are subspaces of the larger subspace that the  $S_c > 0$  vacuum of Eq. (23) refers to. Alike in Ref.<sup>2</sup>, let us divide the Hilbert space of the model (1) in a set of subspaces spanned by the states with constant values of  $S_c$ ,  $S_\eta$ , and  $S_s$  and hence also of  $N_c = 2S_c$ ,  $M_\eta = N_{a_\eta}^D = [N_a^D - 2S_c]$ , and  $M_s = N_{a_s}^D = 2S_c$ . We recall that for the subspace with constant values of  $S_c$ ,  $S_\eta$ , and  $S_s$  under consideration  $M_\eta = N_{a_\eta}^D$  (and  $M_s = N_{a_s}^D$ ) is both the total number of  $\eta$ -spinons (and spinons) and the number of sites of the  $\eta$ -spin (and spin) effective lattice.

According to the studies of Ref.<sup>2</sup> the dimension of each such a subspace is,

$$d_r \cdot \prod_{\alpha=\eta,s} \mathcal{N}(S_\alpha, M_\alpha), \quad (48)$$

where  $d_r$  and  $\mathcal{N}(S_\alpha, M_\alpha)$  are given by,

$$d_r = \binom{N_a^D}{2S_c}; \quad \mathcal{N}(S_\alpha, M_\alpha) = (2S_\alpha + 1) \left\{ \binom{M_\alpha}{M_\alpha/2 - S_\alpha} - \binom{M_\alpha}{M_\alpha/2 - S_\alpha - 1} \right\}, \quad (49)$$



and are the number of  $U(1)$  symmetry state representations and that of  $\eta$ -spin  $SU(2)$  ( $\alpha = \eta$ ) or spin  $SU(2)$  ( $\alpha = s$ ) symmetry state representations, respectively.

The dimension  $d_r$  given in Eq. (49) is here straightforwardly recovered as  $d_r = \binom{N_a^D}{N_c^D}$  and equals the number of occupancy configurations of the  $N_c = 2S_c$   $c$  fermions in their  $c$  band with  $N_a^D$  discrete momentum values. On the other hand, the values of the numbers  $N_{a\nu}^D$  of discrete momentum values of the  $\alpha\nu$  band must obey exactly the following equality for all subspaces,

$$\frac{\mathcal{N}(S_\alpha, M_\alpha)}{(2S_\alpha + 1)} = \sum_{\{N_{\alpha\nu}\}} \prod_{\nu=1}^{C_\alpha} \binom{N_{a\nu}^D}{N_{\alpha\nu}}, \quad \alpha = \eta, s. \quad (50)$$

Here  $\binom{N_{a\nu}^D}{N_{\alpha\nu}}$  is the number of occupancy configurations of the  $N_{\alpha\nu}$   $\alpha\nu$  fermions in their  $\alpha\nu$  band with  $N_{a\nu}^D$  discrete momentum values and the  $\{N_{\alpha\nu}\}$  summation runs over all sets of  $N_{\alpha\nu}$  numbers for  $\nu = 1, 2, \dots, C_\alpha$  that owing to the conservation of  $C_\alpha$  exactly obey the subspace sum-rule,

$$2C_\alpha = \sum_{\nu=1}^{C_\alpha} 2\nu N_{\alpha\nu} = [M_\alpha - 2S_\alpha], \quad \alpha = \eta, s. \quad (51)$$

The general expression of the number  $N_{a\nu}^D$  of  $\alpha\nu$  band discrete momentum values that obeys Eq. (50) for all subspaces corresponds indeed to that given in Eq. (42). Consistently, the occupancies of the independent  $\eta$ -spinons and independent spinons give rise to the usual factors  $(2S_\eta + 1)$  and  $(2S_s + 1)$ , respectively, appearing in the expressions provided in Eqs. (49) and (50) for the dimensions  $\mathcal{N}(S_\eta, M_\eta)$  and  $\mathcal{N}(S_s, M_s)$ . In Appendix C it is shown that the subspace-dimension summation,

$$\mathcal{N}_{tot} = \sum_{S_c=0}^{[N_a^D/2]} \sum_{S_\eta=0}^{[N_a^D/2-S_c]} \sum_{S_s=0}^{S_c} \binom{N_a^D}{2S_c} \prod_{\alpha=\eta,s} \frac{[1 + (-1)^{2S_\alpha+2S_c}]}{2} \mathcal{N}(S_\alpha, M_\alpha) = 4^{N_a^D}, \quad (52)$$

leads indeed to the dimension  $4^{N_a^D}$  of the full Hilbert space. It follows that the present description in terms of momentum eigenstates is complete.

In the  $N_a^D \gg 1$  limit considered here and alike for the  $\eta$ -spin and spin effective lattices, provided that  $N_{a\nu}^D/N_a^D$  is finite the related  $\alpha\nu$  effective lattices can for 1D and 2D be represented by 1D and square lattices, respectively, of lattice constant,

$$a_{\alpha\nu} = \frac{L}{N_{a\nu}^D} = \frac{N_a}{N_{a\nu}^D} a = \frac{N_{a\alpha}}{N_{a\nu}^D} a_\alpha; \quad N_{a\nu}^D \geq 1, \quad (53)$$

where  $\nu = 1, \dots, C_\alpha$  and  $\alpha = \eta, s$ . In turn, the corresponding  $\alpha\nu$  bands whose number of discrete momentum values is also given by  $N_{a\nu}^D$  are well defined even when  $N_a^D$  is given by a finite small number,  $N_a^D = 1, 2, 3, \dots$

For the model on the square lattice and states with numbers  $N_{\alpha\nu} = N_{a\nu}^2$  for  $\alpha\nu \neq s1$  and  $N_{s1} \approx N_{a_{s1}}^2$  for  $\alpha\nu = s1$  where  $[N_{a_{s1}}^2 - N_{s1}]$  vanishes or is of order  $1/N_a^2$  for  $N_a^2 \rightarrow \infty$ , the lattice constant  $a_{\alpha\nu}$  is directly related to the fictitious magnetic-field length  $l_{\alpha\nu}$  associated with the field of Eq. (25). Indeed, in that case one has that  $\langle n_{\vec{r}_j, \alpha\nu} \rangle \approx 1$  and such a fictitious magnetic field reads  $\vec{B}_{\alpha\nu}(\vec{r}_j) \approx \Phi_0 \sum_{j' \neq j} \delta(\vec{r}_{j'} - \vec{r}_j) \vec{e}_{x_3}$ . It acting on one  $\alpha\nu$  fermion differs from zero only at the positions of other  $\alpha\nu$  fermions. In the mean field approximation one replaces it by the average field created by all  $\alpha\nu$  fermions at position  $\vec{r}_j$ . This gives,  $\vec{B}_{\alpha\nu}(\vec{r}_j) \approx \Phi_0 n_{\alpha\nu}(\vec{r}_j) \vec{e}_{x_3} \approx \Phi_0 [N_{a\nu}^2/L^2] \vec{e}_{x_3} = [\Phi_0/a_{\alpha\nu}^2] \vec{e}_{x_3}$ . One then finds that the number  $N_{a\nu}^2$  of the  $\alpha\nu$  band discrete momentum values equals  $[B_{\alpha\nu} L^2]/\Phi_0$  and the  $\alpha\nu$  effective lattice spacing  $a_{\alpha\nu}$  is expressed in terms to the fictitious magnetic-field length  $l_{\alpha\nu}$  as  $a_{\alpha\nu}^2 = 2\pi l_{\alpha\nu}^2$ . This is consistent with for such states each  $\alpha\nu$  fermion having a flux tube of one flux quantum on average attached to it. For the states under consideration the  $\alpha\nu$  fermion problem is related to the Chern-Simons theory<sup>36</sup>, the number of flux quanta being one being consistent with the  $\alpha\nu$  fermion and  $\alpha\nu$  bond-particle wave functions obeying Fermi and Bose statistics, respectively. Hence the composite  $\alpha\nu$  fermion consists of  $2\nu$   $\eta$ -spinons ( $\alpha = \eta$ ) or spinons ( $\alpha = s$ ) plus an infinitely thin flux tube attached to it.

The states that span the one- and two-electron subspace belong to such a class of states so that for the model on the square lattice in that subspace the composite  $s1$  fermion consists of two spinons in a spin-singlet configuration plus an infinitely thin flux tube attached to it<sup>1</sup>. Thus, each  $s1$  fermion appears to carry a fictitious magnetic solenoid with it as it moves around in the  $s1$  effective lattice. Finally, since for such a quantum liquid the  $s1$  fermions play a major

role we find from straightforward manipulations of Eqs. (42) and (43) for  $\alpha\nu = s1$  that the number  $N_{as1}^D = [N_{s1} + N_{s1}^h]$  of  $s1$  effective lattice sites and thus of  $s1$  band discrete momentum values is given by,

$$N_{as1}^D = [S_c + S_s + \sum_{\nu=3}^{C_s} (\nu - 2) N_{s\nu}]. \quad (54)$$

Hence for a subspace where  $N_{s\nu} = 0$  for  $\nu \geq 3$  one has that  $N_{as1}^D = [S_c + S_s]$  is a good quantum number.

## E. The momentum eigenstates of our description and the good and quasi-good quantum numbers

### 1. The momentum eigenstates of our description

The low-energy physics of a 3D perturbative and isotropic many-electron system for which each energy eigenstate  $|\Psi(0)\rangle$  of the corresponding non-interacting system evolves upon adiabatically switching on the interaction  $U$  on an energy eigenstate  $|\Psi(U)\rangle$  is in general successfully described by Fermi liquid theory<sup>28</sup>. (In contrast to the Hubbard model, here the interaction  $U$  is not necessarily onsite.) Since the two sets of orthogonal and normalized states  $\{|\Psi(0)\rangle\}$  and  $\{|\Psi(U)\rangle\}$  are complete and refer to the same Hilbert space, there is a well-defined unitary transformation such that for each  $U = 0$  energy eigenstate  $|\Psi(0)\rangle$  there is exactly one  $U > 0$  energy eigenstate  $|\Psi(U)\rangle = \hat{\mathcal{V}}^\dagger |\Psi(0)\rangle$  where  $\hat{\mathcal{V}}^\dagger = \hat{\mathcal{V}}^\dagger(U)$  is the corresponding unitary operator. For the exact ground state such a statement is equivalent to the Gell-Mann and Low theorem<sup>44</sup>. By perturbative system we mean above that  $\langle \Psi(0) | \Psi(U) \rangle \neq 0$  for all such pairs of states of each of the two complete sets.

If the  $U = 0$  energy eigenstates can be written as Slater determinants of the form,

$$|\Psi(0)\rangle = \prod_{\sigma} \prod_{\vec{k}} c_{\vec{k},\sigma}^\dagger |0\rangle, \quad (55)$$

where  $c_{\vec{k},\sigma}^\dagger$  creates an electron of momentum  $\vec{k}$  and spin projection  $\sigma$  and  $|0\rangle$  is the electronic vacuum, then the corresponding states  $|\Psi(U)\rangle = \hat{\mathcal{V}}^\dagger |\Psi(0)\rangle$  read,

$$|\Psi(U)\rangle = \prod_{\sigma} \prod_{\vec{k}} \hat{\mathcal{V}}^\dagger c_{\vec{k},\sigma}^\dagger |0\rangle = \prod_{\sigma} \prod_{\vec{k}} [\hat{\mathcal{V}}^\dagger c_{\vec{k},\sigma}^\dagger \hat{\mathcal{V}}] \hat{\mathcal{V}}^\dagger |0\rangle = \prod_{\sigma} \prod_{\vec{k}} \tilde{c}_{\vec{k},\sigma}^\dagger |0\rangle; \quad \tilde{c}_{\vec{k},\sigma}^\dagger = \hat{\mathcal{V}}^\dagger c_{\vec{k},\sigma}^\dagger \hat{\mathcal{V}}; \quad \hat{\mathcal{V}}^\dagger |0\rangle = |0\rangle. \quad (56)$$

Here  $\tilde{c}_{\vec{k},\sigma}^\dagger = \hat{\mathcal{V}}^\dagger c_{\vec{k},\sigma}^\dagger \hat{\mathcal{V}}$  is the creation operator of a quasiparticle of momentum  $\vec{k}$  and spin projection  $\sigma$ .

Note that since for  $U/4t \rightarrow 0$  the unitary operator  $\hat{\mathcal{V}}^\dagger$  becomes the unit operator, a state  $|\Psi(0)\rangle$  of Eq. (55) equals the corresponding state  $|\Psi(U)\rangle$  of Eq. (56) for  $U/4t \rightarrow 0$ . Let us consider the one-electron Green function,

$$G(\vec{k}, \sigma, t - t') = -i \langle \Psi_{GS}(U) | T c_{\vec{k},\sigma}(t) c_{\vec{k},\sigma}^\dagger(t') | \Psi_{GS}(U) \rangle, \quad (57)$$

where for  $U > 0$  (and  $U = 0$ ) the  $N + 1$  states  $c_{\vec{k},\sigma}^\dagger(t) |\Psi_{GS}(U)\rangle$  and  $c_{\vec{k},\sigma}^\dagger(t') |\Psi_{GS}(U)\rangle$  and  $N - 1$  states  $c_{\vec{k},\sigma}(t) |\Psi_{GS}(U)\rangle$  and  $c_{\vec{k},\sigma}(t') |\Psi_{GS}(U)\rangle$  are not (and are) energy eigenstates. In turn, for  $U > 0$  the “ $N + 1$  quasiparticle states”  $\tilde{c}_{\vec{k},\sigma}^\dagger(t) |\Psi_{GS}(U)\rangle$  and  $\tilde{c}_{\vec{k},\sigma}^\dagger(t') |\Psi_{GS}(U)\rangle$  and “ $N - 1$  quasiparticle states”  $\tilde{c}_{\vec{k},\sigma}(t) |\Psi_{GS}(U)\rangle$  and  $\tilde{c}_{\vec{k},\sigma}(t') |\Psi_{GS}(U)\rangle$  are energy eigenstates, yet they cannot be proved in real experiments because only the electrons are physical particles. Indeed, quasiparticles exist only inside the many-electron system. Therefore, quasiparticles can only be added to or removed from the system upon addition to and removal from it of electrons. That for  $U > 0$  the above one-electron states are not energy eigenstates implies that the renormalization factor  $Z(\vec{k})$  is smaller than one and for momenta  $\vec{k}$  in the vicinity of the isotropic Fermi surface and small excitation energy  $\omega$  such states have an inverse lifetime proportional to  $\omega^2$  so that the “quasiparticle lifetime” is finite for  $\omega > 0$  and becomes infinite as  $\omega \rightarrow 0$ <sup>28</sup>.

We emphasize that in spite of such an one-electron lifetime being finite, the quasiparticle occupancy configurations (56) generate for  $U > 0$  exact energy eigenstates, whose continuous changes with time occur according to the many-electron Schrödinger equation. Concerning one- and two-electron excitations, the concept of a quasiparticle is well-defined for low-energy eigenstates whose quasiparticle occupancy configurations differ from those of the initial ground state only near the Fermi surface. In turn, in the absence of one- and two-electron quantum measurement processes the quasiparticle occupancy configurations (56) as defined here generate all  $U > 0$  energy eigenstates. Hence solution of the quantum problem is equivalent to derivation of the unitary operator  $\hat{\mathcal{V}}^\dagger = \hat{\mathcal{V}}^\dagger(U)$  for  $U > 0$ . Unfortunately,

this is in general a very involved and unsolved problem. Landau's Fermi liquid theory is a very useful scheme that allows solution of it for the subspace spanned by excited energy eigenstates generated from the initial  $U > 0$  ground state by a finite number of quasiparticle processes near the Fermi surface.

In turn, for the Hubbard model on the square or 1D lattices our choice of  $4^{N_a^D}$  energy eigenstates  $\{|\Psi_\infty\rangle\}$  for  $U/4t \rightarrow \infty$  reported is, as in Subsection II-A, such that the states  $|\Psi_{U/4t}\rangle = \hat{V}^\dagger |\Psi_\infty\rangle$  are energy eigenstates for finite values  $U/4t > 0$ . Following the result of Appendix A that the general problem of that model in the whole Hilbert space can be fully described by the same model in the LWS subspace, for simplicity to start with our discussion refers to that subspace. That just means that for states with independent  $\eta$ -spinon and/or independent spinon occupancy the  $\eta$ -spin and spin projection, respectively, of such objects is given by  $+1/2$ . Within our operator description for the model on the square lattice each of the  $U/4t \rightarrow \infty$  LWS energy eigenstates of the corresponding set  $\{|\Psi_{LWS;\infty}\rangle\}$  can be expressed as a suitable superposition of  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates  $\{|\Phi_{LWS;\infty}\rangle\}$  with the same values for such physical quantities and also for the numbers  $C_\alpha = \sum_{\nu=1}^{C_\alpha} \nu N_{\alpha\nu}$  of Eqs. (20), (21), (31), and (47) where  $\alpha = \eta, s$ . The latter states can be generated by occupancy configurations of the microscopic momenta  $\vec{q}$  carried by the  $c$  and  $\alpha\nu$  fermions, which as justified below are of the general form,

$$|\Phi_{LWS;\infty}\rangle = [\prod_{\alpha} \prod_{\nu} \prod_{\vec{q}'} \mathcal{F}_{\vec{q}',\alpha\nu}^\dagger |0_\alpha; N_{a_\alpha^D}\rangle] [\prod_{\vec{q}} \mathcal{F}_{\vec{q},c}^\dagger |GS_c; 0\rangle]. \quad (58)$$

Here  $\mathcal{F}_{\vec{q}',\alpha\nu}^\dagger$  and  $\mathcal{F}_{\vec{q},c}^\dagger$  are creation operators of a  $U/4t \rightarrow \infty$   $\alpha\nu$  fermion of momentum  $\vec{q}'$  and  $c$  fermion of momentum  $\vec{q}$ , respectively, and the  $\eta$ -spin  $SU(2)$  vacuum  $|0_\eta; N_{a_\eta}^D\rangle$  associated with  $N_{a_\eta}^D$  independent  $+1/2$   $\eta$ -spinons, the spin  $SU(2)$  vacuum  $|0_s; N_{a_s}^D\rangle$  with  $N_{a_s}^D$  independent  $+1/2$  spinons, and the  $c$   $U(1)$  vacuum  $|GS_c; 0\rangle$  such that  $\prod_{\vec{q}} \mathcal{F}_{\vec{q},c}^\dagger |GS_c; 0\rangle = |GS_c; 2S_c\rangle$  has  $N_c = 2S_c$   $c$  fermions are those of the vacuum given in Eq. (23). We recall that for  $U/4t \rightarrow \infty$  Eqs. (8)-(17) are equivalent to Eqs. (1)-(3) of Ref.<sup>12</sup> with the  $c$  fermion creation operator  $f_{\vec{r}_j,c}^\dagger$  replaced by the quasicharge annihilation operator  $\hat{c}_r$ . Therefore, the operator  $\mathcal{F}_{\vec{q},c}^\dagger$  is given by,

$$\mathcal{F}_{\vec{q},c}^\dagger = \frac{1}{\sqrt{N_a^D}} \sum_r e^{+i\vec{q}\cdot\vec{r}} \hat{c}_r, \quad (59)$$

where within the notation of Ref.<sup>12</sup>,  $r \equiv \vec{r}_j$  are the real-space coordinates of the quasicharge particles of that reference. The holes of such quasicharge particles are for  $U/4t \rightarrow \infty$  the spinless fermions that describe the charge degrees of freedom of the electrons of the singly occupied sites. Moreover, the spinons and  $\eta$ -spinons of the  $2\nu$ -spinon operators  $\mathcal{F}_{\vec{q}',s\nu}^\dagger$  and  $2\nu$ - $\eta$ -spinon operators  $\mathcal{F}_{\vec{q}',\eta\nu}^\dagger$ , respectively, are associated with the local spin and pseudospin operators, respectively, defined in that reference. As discussed in Appendix B, for the 1D model all states (58) are energy eigenstates<sup>1</sup>, so that  $|\Psi_{LWS;\infty}\rangle = |\Phi_{LWS;\infty}\rangle$ . For the model on the square lattice that holds only for some of these states. For instance, it holds for the energy eigenstates that span the one- and two-electron subspace as defined below so that  $|\Psi_{LWS;\infty}\rangle = |\Phi_{LWS;\infty}\rangle$  for that subspace.

Symmetry implies that for the Hubbard model on a square lattice at  $U/4t > 0$  the  $N_{a_{\alpha\nu}}^2$   $\alpha\nu$  band discrete momentum values are  $U/4t$  independent for states belonging to the same  $V$  tower. Importantly, the vacua of the  $U/4t \rightarrow \infty$  states (58) are invariant under the electron - rotated-electron unitary transformation so that for finite values of  $U/4t$  the corresponding  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates read,

$$|\Phi_{LWS;U/4t}\rangle = [\prod_{\alpha} \prod_{\nu} \prod_{\vec{q}'} f_{\vec{q}',\alpha\nu}^\dagger |0_\alpha; N_{a_\alpha^D}\rangle] [\prod_{\vec{q}} f_{\vec{q},c}^\dagger |GS_c; 0\rangle]; \quad f_{\vec{q}',\alpha\nu}^\dagger = \hat{V}^\dagger \mathcal{F}_{\vec{q}',\alpha\nu}^\dagger \hat{V}; \quad f_{\vec{q},c}^\dagger = \hat{V}^\dagger \mathcal{F}_{\vec{q},c}^\dagger \hat{V}. \quad (60)$$

Alike in the  $U/4t \rightarrow \infty$  limit, for the one- and two-electron subspace the energy eigenstates  $|\Psi_{LWS;U/4t}\rangle$  of the model on the square lattice are such that  $|\Psi_{LWS;U/4t}\rangle = |\Phi_{LWS;U/4t}\rangle$ , whereas for the 1D model the equality  $|\Psi_{LWS;U/4t}\rangle = |\Phi_{LWS;U/4t}\rangle$  holds for all  $U/4t > 0$  energy eigenstates<sup>1,37</sup>. In Appendix B it is confirmed that the discrete momentum values of the  $c$  and  $\alpha\nu$  fermion operators appearing on the right-hand side of Eq. (60) are indeed the good quantum numbers of the exact solution whose occupancy configurations generate the energy eigenstates. Furthermore, in that Appendix the relation of the  $c$  and  $\alpha\nu$  fermion operators whose suitable products refer to the operators whose application onto the theory vacua generates the states (60) to the creation and annihilation fields of the charge ABCDF algebra<sup>16</sup> and more traditional spin ABCD Faddeev-Zamolodchikov algebra<sup>24</sup> of the algebraic formulation of the 1D exact solution of Ref.<sup>16</sup> is discussed and the consistency between the two corresponding operational representations confirmed.

We recall that addition of chemical-potential and magnetic-field operator terms to the Hamiltonian (1) lowers its symmetry. However, such operator terms commute with that Hamiltonian and the momentum operator so that its

energy and momentum eigenstates correspond to state representations of the  $SO(3) \times SO(3) \times U(1)$  group for all values of the densities  $n = (1 - x)$  and  $m$ . The same holds for the  $4^{N_a^D}$  momentum eigenstates considered here, whose  $c$  fermion and  $\alpha\nu$  fermion occupancy configurations and independent  $\eta$ -spinon and spinon occupancies are of the form,

$$|\Phi_{U/4t}\rangle = \prod_{\alpha=\eta,s} \frac{(\hat{S}_\alpha^\dagger)^{L_\alpha, -1/2}}{\sqrt{\mathcal{C}_\alpha}} |\Phi_{LWS;U/4t}\rangle = \prod_{\alpha} \frac{(\hat{S}_\alpha^\dagger)^{L_\alpha, -1/2}}{\sqrt{\mathcal{C}_\alpha}} \prod_{\nu} \prod_{\vec{q}'} f_{\vec{q}',\alpha\nu}^\dagger |0_\alpha; N_{a_\alpha^D}\rangle \left[ \prod_{\vec{q}} f_{\vec{q},c}^\dagger |GS_c; 0\rangle \right]. \quad (61)$$

Such states correspond indeed to the state representations of the  $SO(3) \times SO(3) \times U(1)$  group. In this expression  $|\Phi_{LWS;U/4t}\rangle$  are the states of Eq. (60) and the normalization constant  $\mathcal{C}_\alpha$  is given in Eq. (A2) of Appendix A. The set of  $4^{N_a^D}$  momentum eigenstates of form (61) is complete and corresponds exactly to the  $c$  fermion and  $\alpha\nu$  momentum occupancy configurations associated with the subspace dimensions of Eq. (48) and the corresponding subspace dimensions,

$$d_r \cdot \prod_{\alpha=\eta,s} (2S_\alpha + 1) \cdot \mathcal{N}(S_\alpha, M_\alpha), \quad (62)$$

where  $d_r$  and  $\mathcal{N}(S_\alpha, M_\alpha)$  are given in Eq. (49) and here we have accounted for the occupancies of the independent  $\eta$ -spinons and independent spinons associated with the usual factors  $(2S_\eta + 1)$  and  $(2S_s + 1)$ , respectively. Use of the summations of the subspace dimensions of Eq. (62) performed in Appendix C confirms that the correct Hilbert space dimension  $4^{N_a^D}$  is indeed obtained. (For the 1D model one has that such  $4^{N_a^D}$  states  $\{|\Phi_{U/4t}\rangle\}$  are both momentum and energy eigenstates so that  $|\Psi_{U/4t}\rangle = |\Phi_{U/4t}\rangle$ .)

For the the operators  $f_{\vec{q}_j,\alpha\nu}^\dagger$  there is an independent problem for the model in each subspace with constant values of  $S_c$ ,  $S_s$ , and number of sites of the  $\alpha\nu$  effective lattice and discrete momentum values of the  $\alpha\nu$  band  $N_{a_{\alpha\nu}}^D = [N_{\alpha\nu} + N_{\alpha\nu}^h]$  given in Eq. (42). Hence the operators  $f_{\vec{q}_j,\alpha\nu}^\dagger$  and  $f_{\vec{q}_j,\alpha\nu}$  act onto such subspaces, where they are the building blocks of the generators that change the  $\alpha\nu$  fermion occupancy configurations. Hence and as mentioned above, such operators act onto subspaces spanned by mutually neutral states and that assures that for the model on the square lattice the components  $q_{x1}$  and  $q_{x2}$  of the microscopic momenta  $\vec{q} = [q_{x1}, q_{x2}]$  refer to commuting  $s1$  translation generators  $\hat{q}_{s1\ x1}$  and  $\hat{q}_{s1\ x2}$ <sup>36</sup>. In turn, for the operators  $f_{\vec{q}_j,c}^\dagger$  there are in 1D two types of quantum problems depending on the even or odd character of the number  $[B_\eta + B_s] = \sum_{\alpha,\nu} N_{\alpha\nu}$ . Indeed, in spite of the  $c$  effective lattice being identical to the original lattice for the whole Hilbert space, as discussed in Appendix B the  $c$  fermions feel the Jordan-Wigner phases of the  $\alpha\nu$  fermions created or annihilated under subspace transitions that change the number  $[B_\eta + B_s]$ . Hence for 1D the  $c$  band discrete momenta have different values for  $[B_\eta + B_s]$  odd and even, respectively. Also for the model on the square lattice the  $c$  fermions feel the Jordan-Wigner phases of the  $\alpha\nu$  fermions created or annihilated under subspace transitions that change the number  $[B_\eta + B_s]$ <sup>1</sup>.

The generators that transform into each other the states with constant values of  $S_c$ ,  $S_s$ , and  $N_{a_{\alpha\nu}}^D = [N_{\alpha\nu} + N_{\alpha\nu}^h]$ , which span such a subspace, can be expressed in terms of creation and annihilation  $\alpha\nu$  fermion operators. These states can be formally written as given in Eqs. (60) and (61) provided that the  $\alpha\nu$  momentum bands are those of the state under consideration. The  $\alpha\nu$  fermion operators  $f_{\vec{q},\alpha\nu}^\dagger$  and  $f_{\vec{q},\alpha\nu}$  act onto subspaces spanned by neutral states. However, creation of one  $\alpha\nu$  fermion is a well-defined process whose generator is the product of an operator that fulfills small changes in the  $\alpha\nu$  effective lattice and corresponding  $\alpha\nu$  momentum band and the operator  $f_{\vec{q},\alpha\nu}^\dagger$  appropriate to the excited-state subspace. Since in the case of Eqs. (60) and (61) it is assumed the  $\alpha\nu$  momentum bands are those of the state under consideration the corresponding generators on the vacua are simple products of  $f_{\vec{q},\alpha\nu}^\dagger$  operators, as given in these equations.

As discussed in Appendix B, the use of the exact solution confirms that for 1D the states (60) and (61) are momentum and energy eigenstates. Following the way that our operator description is constructed they are momentum eigenstates of the model on the square lattice as well. This is consistent with general properties that play a key role in the model physics: Both for the 1D and square lattices and in contrast to the Hamiltonian (1), the momentum operator commutes with the set of  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu}$  of Eq. (27) and unitary operator  $\hat{V}$  associated with the electron - rotated-electron unitary transformation. Since the Hamiltonian does not commute with the  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu}$ , the  $\alpha\nu$  fermion operators labelled by the  $\alpha\nu$  band discrete momentum values  $\vec{q}_j$  where  $j = 1, \dots, N_{a_{\alpha\nu}}^2$  act onto and are defined in subspaces with constant values of  $N_{a_{\alpha\nu}}^2$ , and the values of their discrete momenta are subspace dependent, the microscopic momenta  $\vec{q}_j$  of such objects are not in general conserved. Consistently, the states of Eqs. (60) and (61) generated by momentum occupancy configurations of such  $\alpha\nu$  fermions are not in general energy eigenstates.

The unitary operator  $\hat{V}^\dagger$  considered in Subsection II-A has been constructed to inherently generating exact  $U/4t > 0$  energy and momentum eigenstates  $|\Psi_{LWS;U/4t}\rangle = \hat{V}^\dagger |\Psi_{LWS;\infty}\rangle$  and  $|\Psi_{U/4t}\rangle = \hat{V}^\dagger |\Psi_\infty\rangle =$

$\prod_{\alpha}[(\hat{S}_{\alpha}^{\dagger})^{L_{\alpha,-1/2}/\sqrt{C_{\alpha}}}|\Psi_{LWS;U/4t}\rangle$ . For the model on the square lattice the energy and momentum eigenstates  $|\Psi_{U/4t}\rangle$  are within our description a well-defined superposition of momentum eigenstates  $|\Phi_{U/4t}\rangle$  of Eq. (61) of equal  $S_{\eta}$ ,  $S_{\eta}^z$ ,  $S_s$ ,  $S_s^z$ , and  $S_c$  values and momentum eigenvalue. The energy eigenvalues of the former states are  $U/4t$  dependent. In turn, the invariance of the momentum operator under  $\hat{V}$  imposes that the momentum eigenvalues of both the states  $|\Psi_{U/4t}\rangle$  and  $|\Phi_{U/4t}\rangle$  are independent of  $U/4t$ . Therefore, provided that the corresponding set  $\{|\Psi_{\infty}\rangle\}$  of  $U/4t \gg 1$  energy and momentum eigenstates and thus that  $\{|\Phi_{\infty}\rangle\}$  of momentum eigenstates associated with the same unitary operator  $\hat{V}^{\dagger}$  are suitably chosen according to the recipe of Subsection II-A, the momentum eigenvalues of such states are the same as those of the corresponding  $U/4t > 0$  momentum and energy eigenstates  $|\Psi_{U/4t}\rangle = \hat{V}^{\dagger}|\Psi_{\infty}\rangle$  and momentum eigenstates  $|\Phi_{U/4t}\rangle = \hat{V}^{\dagger}|\Phi_{\infty}\rangle$ , respectively.

Hence the rotated electrons used as starting building blocks of the description of the quantum problem in terms of  $c$  fermions,  $\alpha\nu$  fermions, and independent  $\eta$ -spinons and spinons have been constructed to inherently the momentum eigenvalues being for  $U/4t > 0$  fully determined by those of the corresponding  $U/4t \rightarrow \infty$  system. For both the model on the square and 1D lattices it follows from Eqs. (26) and (27) that the momentum eigenvalues are indeed independent of  $U/4t$  and given by,

$$\vec{P} = \sum_{\vec{q}} \vec{q}_j N_c(\vec{q}) + \sum_{\nu=1}^{C_s} \sum_{\vec{q}} \vec{q} N_{s\nu}(\vec{q}) + \sum_{\nu=1}^{C_{\eta}} \sum_{\vec{q}} [\vec{\pi} - \vec{q}] N_{\eta\nu}(\vec{q}) + \vec{\pi} M_{\eta,-1/2}. \quad (63)$$

Here  $N_c(\vec{q})$  and  $N_{\alpha\nu}(\vec{q})$  are the expectation values of the momentum distribution-function operators (28). For the model on the 1D lattice the  $c$  and  $\alpha\nu$  fermion discrete momentum values are good quantum numbers so that the momentum distribution functions  $N_c(q)$  and  $N_{\alpha\nu}(q)$  are eigenvalues of the operators (28) and have values 1 and 0 for occupied and unoccupied momentum values, respectively<sup>1,37</sup>. As justified below, for the model on the square lattice that remains true for  $N_c(\vec{q})$  and for such a model in the one- and two-electron subspace defined in Section V this is true for  $N_{s1}(\vec{q})$  as well.

For  $D = 1$  the validity of expression (63) is confirmed by the exact solution<sup>1,37</sup>. Let us provide further information on why for the Hubbard model on the square lattice the momentum operator can for  $U/4t > 0$  be expressed as given in Eqs. (26) and (27) so that the momentum eigenvalues are of the general form (63), alike for the 1D model. For  $U/t \rightarrow \infty$  electron single and doubly occupancy become good quantum numbers so that the electrons that singly occupy sites do not feel the on-site repulsion. That implies that the discrete momentum values  $\vec{q}$  associated with their occupancy configurations separate into (i) those associated with electron hopping, which are good quantum numbers and involve the charge degrees of freedom and finite kinetic energy and are carried by the  $c$  fermions and (ii) those associated with the  $\eta$ -spinon and spinons, including the composite  $\eta\nu$  and  $s\nu$  fermion occupancy configurations, respectively, whose momentum bands are for  $U/t \rightarrow \infty$  dispersionless.

That for the model on the square lattice the momentum eigenvalues have for  $U/4t > 0$  the general form,

$$\vec{P} = \sum_{\vec{q}} \vec{q} N_c(\vec{q}) + \vec{P}_{\eta-spin} + \vec{P}_{spin}, \quad (64)$$

where  $\vec{P}_{\eta-spin}$  and  $\vec{P}_{spin}$  are the momentum contributions associated with the  $\eta$ -spin and spin configurations, respectively, which for  $U/t \rightarrow \infty$  do not contribute to the kinetic energy, is an exact result. Indeed, in that limit the rotated electrons are the electrons, which for the finite-energy physics can only singly occupy sites and due to the exclusion principle behave as spinless and  $\eta$ -spinless fermions. Since the only effect of the interactions on their charge degrees of freedom is to impose such a single occupancy constrain, those lead to a momentum contribution  $\sum_{\sigma} \sum_{\vec{q}} \vec{q} N_{\sigma}(\vec{q}) = \sum_{\vec{q}} \vec{q} N(\vec{q})$  where  $N(\vec{q}) = \sum_{\sigma} N_{\sigma}(\vec{q})$  is the  $U/t \rightarrow \infty$  electron momentum distribution and  $N_{\sigma}(\vec{q}) = \langle \Psi_{\infty} | c_{\vec{q},\sigma}^{\dagger} c_{\vec{q},\sigma} | \Psi_{\infty} \rangle$ . In that limit one then has  $N_c(\vec{q}) = N(\vec{q})$ . For  $U/4t$  finite the  $U/t \rightarrow \infty$  distribution  $N(\vec{q})$  is replaced by the rotated-electron momentum distribution,

$$N_{rot}(\vec{q}) = \sum_{\sigma} \langle \Psi_{U/4t} | \tilde{c}_{\vec{q},\sigma}^{\dagger} \tilde{c}_{\vec{q},\sigma} | \Psi_{U/4t} \rangle = \sum_{\sigma} \langle \Psi_{\infty} | \hat{V} [\hat{V}^{\dagger} c_{\vec{q},\sigma}^{\dagger} \hat{V} \hat{V}^{\dagger} c_{\vec{q},\sigma} \hat{V}] \hat{V}^{\dagger} | \Psi_{\infty} \rangle = \sum_{\sigma} \langle \Psi_{\infty} | c_{\vec{q},\sigma}^{\dagger} c_{\vec{q},\sigma} | \Psi_{\infty} \rangle, \quad (65)$$

and the  $c$  fermion momentum distribution reads  $N_c(\vec{q}) = N_{rot}(\vec{q})$ . Indeed, for rotated electrons singly occupancy remains a good quantum number for  $U/4t > 0$  and the  $c$  effective lattice occupied sites have exactly the same spatial variables as the sites singly occupied by rotated electrons in the original lattice.

For the model on the square lattice an energy eigenstate  $|\Phi_{U/4t}\rangle$  is a superposition of  $S_{\eta}$ ,  $S_{\eta}^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates  $|\Phi_{U/4t}\rangle$  of Eq. (61) with the same momentum eigenvalue,  $S_{\eta}$ ,  $S_{\eta}^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$  values, and  $c$  fermion momentum distribution function  $N_c(\vec{q}) = N_{rot}(\vec{q})$ . Hence all states  $|\Phi_{U/4t}\rangle$  of such a set have the same distribution function  $N_c(\vec{q}) = \sum_{\sigma} \langle \Phi_{U/4t} | \tilde{c}_{\vec{q},\sigma}^{\dagger} \tilde{c}_{\vec{q},\sigma} | \Phi_{U/4t} \rangle$ . As discussed below, consistently with the commutator of

the Hamiltonian with the  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu}$  of Eq. (27) not vanishing, such states differ in general in the  $\alpha\nu$  fermion momentum occupancies. Since for momentum eigenstates  $|\Phi_{U/4t}\rangle = \hat{V}^\dagger|\Phi_\infty\rangle$  of Eq. (61) (one for each value of  $U/4t > 0$ ) belonging to the same  $V$  tower the momentum eigenvalues are independent of  $U/4t$ , the contribution to the momentum of the  $c$  fermions is  $\sum_{\vec{q}} \vec{q} N_c(\vec{q})$  where alike in Eq. (65) the distribution function  $N_c(\vec{q}) = N_{rot}(\vec{q}) = \sum_{\sigma} \langle \Phi_{U/4t} | \hat{c}_{\vec{q},\sigma}^\dagger \hat{c}_{\vec{q},\sigma} | \Phi_{U/4t} \rangle$  has for  $U/4t > 0$  the same magnitude  $N(\vec{q}) = \sum_{\sigma} \langle \Phi_\infty | \hat{c}_{\vec{q},\sigma}^\dagger \hat{c}_{\vec{q},\sigma} | \Phi_\infty \rangle$  as for the corresponding  $U/4t \rightarrow \infty$  initial momentum eigenstate  $|\Phi_\infty\rangle$ .

This holds both for the model on the 1D and square lattices. For the model on the former lattice the electron momentum distribution  $N(q)$  is for the  $x = 0$  and  $m = 0$  ground state plotted for  $U/t \rightarrow \infty$  in Fig. 3 (a) of Ref.<sup>45</sup>. Note that the energy spectrum depends on  $U/4t$  so that for the model on the square lattice the  $x > 0$  and  $m = 0$  ground states may belong to different  $V$  towers for different values of  $U/4t$ . The exception is the  $x = 0$  and  $m = 0$  ground state, which belongs to the same  $V$  tower for all  $U/4t > 0$  values, as confirmed in Ref.<sup>1</sup>.

The above analysis confirms that consistently with as given in Eq. (29) the Hamiltonian and momentum operator commute with the  $c$  translation generator  $\hat{q}_c$  of Eq. (27), for  $U/4t > 0$  the distribution  $N_c(\vec{q})$  is an eigenvalue of the operator  $\hat{N}_c(\vec{q})$  of Eq. (28) and has values 1 and 0 for filled and unfilled momentum values, respectively. That result combined with the validity of the momentum spectrum (64) for all occupancy configurations of the  $c$  fermions that generate the momentum eigenstates of form (61) confirms that the discrete momentum values  $\vec{q}$  of the  $c$  fermion band are good quantum numbers for the Hubbard model on the square lattice.

In turn, for  $U/4t \rightarrow \infty$  all  $\eta$ -spin and spin configurations are degenerate and do not contribute to the kinetic energy. Nevertheless they lead to overall momentum contributions  $\vec{P}_{\eta-spin}$  and  $\vec{P}_{spin}$ , respectively. The main point is that the  $\alpha\nu$  fermion operators are defined in and act onto subspaces spanned by mutually neutral states for which for the square-lattice model the  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu x_1}$  and  $\hat{q}_{\alpha\nu x_2}$  commute. That implies that alike in 1D the  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu}$  of Eq. (27) in the presence of the fictitious magnetic field  $\vec{B}_{\alpha\nu}$  of Eq. (25) commute with the momentum operator both in the  $U/4t \rightarrow \infty$  limit and for  $U/4t$  finite, as given in Eq. (29). Consistently with the momentum operator expression provided in Eqs. (26) and (27) and as given in Eq. (63), that then implies that both in the  $U/4t \rightarrow \infty$  limit and for  $U/4t$  finite the momentum contributions  $\vec{P}_{\eta-spin}$  and  $\vec{P}_{spin}$  of Eq. (64) have the form  $\vec{P}_{\eta-spin} = \sum_{\nu} \sum_{\vec{q}} [\vec{\pi} - \vec{q}] N_{\eta\nu}(\vec{q}) + \vec{\pi} M_{\eta,-1/2}$  and  $\vec{P}_{spin} = \sum_{\nu} \sum_{\vec{q}} \vec{q} N_{s\nu}(\vec{q})$ , respectively.

For the Hubbard model on the square lattice the momentum spectrum of Eq. (63) is found in<sup>1</sup> to lead to the correct spin spectrum in some limiting cases. Note however that the momentum area  $N_{\alpha\nu}^2 [2\pi/L]^2$  and discrete momentum values number  $N_{\alpha\nu}^2$  of the  $\alpha\nu$  bands are known. In contrast, the shape of their boundary remains an open issue. The shape of the  $c$  band is the same as that of the first Brillouin zone, yet the discrete momentum values may have small overall shifts under transitions between subspaces with different  $[B_\eta + B_s] = \sum_{\alpha\nu} N_{\alpha\nu}$  values. The studies of Ref.<sup>1</sup> use several approximations to obtain information on the  $c$  and  $s1$  bands momentum values and the corresponding  $c$  and  $s1$  fermion energy dispersions of the model on the square lattice in the one- and two-electron subspace, for which as justified below the  $s1$  fermion discrete momentum values are good quantum numbers.

The square-lattice quantum liquid studied in this paper corresponds to the Hubbard model on the square lattice in such a subspace. For that quantum problem the  $c$  and  $s1$  fermions play the role of “quasiparticles”. There are three main differences relative to an isotropic Fermi liquid<sup>28</sup>: i) Concerning the charge degrees of freedom, the non-interacting limit of the theory refers to  $4t^2/U \rightarrow 0$  rather than to the limit of zero interaction  $U \rightarrow 0$ ; ii) In the  $4t^2/U \rightarrow 0$  limit the  $c$  fermions and  $s1$  fermions become the holes of the “quasicharges” of Ref.<sup>12</sup> and spin-singlet two-spin configurations of the spins of such a reference rather than electrons and only the charge dynamical factor becomes that of non-interacting spinless fermions, the one-electron and spin spectral distributions remaining non-trivial; iii) For  $U/4t > 0$  the  $s1$  band is full and displays a single hole for initial  $m = 0$  ground states and their one-electron excited states, respectively, and as found in Ref.<sup>1</sup> its boundary line is anisotropic, what is behind anomalous one-electron scattering properties<sup>32</sup>.

## 2. The good and quasi-good quantum numbers

That  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ , and  $S_s^z$  are good quantum numbers for both the Hubbard model on the 1D and square lattices implies that the numbers of independent  $\eta$ -spinons ( $\alpha = \eta$ ) and independent spinons ( $\alpha = s$ )  $L_{\alpha, \pm 1/2} = [S_\alpha \mp S_\alpha^z]$  of Eq. (19) are good quantum numbers as well. That the eigenvalue  $S_c$  of the generator of the new  $U(1)$  symmetry of the model global  $SO(3) \times SO(3) \times U(1) = [SU(2) \times SU(2) \times U(1)]/Z_2^2$  symmetry found in Ref.<sup>2</sup> is a good quantum number implies that the numbers  $N_{\alpha s}^D = N_c = M_s = 2S_c$  and  $N_{\alpha \eta}^D = N_c^h = M_\eta = [N_\alpha^D - 2S_c]$  are also good quantum numbers. It then follows that the numbers  $C_\alpha$  of Eqs. (20), (21), (31), and (47), which can be expressed as  $C_\alpha = [N_{\alpha s}^D/2 - S_\alpha]$ , are good quantum numbers as well. The same then applies to the total numbers  $M_{\alpha, \pm 1/2} = L_{\alpha, \pm 1/2} + C_\alpha$  of  $\pm 1/2$   $\eta$ -spinons ( $\alpha = \eta$ ) and  $\pm 1/2$  spinons ( $\alpha = s$ ).

The integrability of the 1D Hubbard model is for  $N_a \rightarrow \infty$  associated with an infinite number of conservation laws such that the Hamiltonian commutes with the infinite  $\alpha\nu$  translation generators  $\vec{q}_{\alpha\nu}$  of Eq. (27) in the presence of the fictitious magnetic fields  $\vec{B}_{\alpha\nu}$ . According to the results of Ref.<sup>46</sup> such laws are equivalent to the independent conservation of the corresponding set of numbers  $\{N_{\alpha\nu}\}$  of  $\alpha\nu$  fermions, which are good quantum numbers. The lack of integrability of the Hubbard model on the square lattice is behind the  $\alpha\nu$  translation generators not commuting with the Hamiltonian and the set of numbers  $\{N_{\alpha\nu}\}$  not being in general good quantum numbers. It follows that for the 1D model the numbers  $B_\alpha$  of Eqs. (44) and (47) and related numbers  $N_{\alpha 1}^h$  and  $N_{s1}$  are good quantum numbers as well, whereas for the model on the square lattice are *quasi-good quantum numbers*. By that we mean that in general they are not good quantum numbers for that model, yet they are good quantum numbers for it defined in the following subspaces:

A)  $B_\eta$  and  $N_{\eta 1}^h$  (and  $B_s$ ,  $N_{s1}^h$ , and  $N_{s1}$ ) are good quantum numbers for the model on the square lattice in subspaces spanned by  $S_\eta = 0$  (and  $S_s = 0$ ) momentum eigenstates provided that  $N_{\eta\nu} > 0$  is finite for a single  $\eta\nu$  branch (and  $N_{s\nu} > 0$  is finite for the  $s1$  branch and a single  $s\nu$  branch other than it) and  $N_{\eta\nu'} = 0$  (and  $N_{s\nu'} = 0$ ) for the remaining  $\eta\nu'$  (and  $s\nu'$ ) branches and  $B_\eta = N_{\eta\nu}$  (and  $[B_s - N_{s1}] = N_{s\nu}$ ) is such that  $2\nu N_{\eta\nu}/N_a^2 \rightarrow 0$  (and  $2\nu N_{s\nu}/N_a^2/N_a^2 \rightarrow 0$  and  $N_{a s1}^2/N_a^2$  is finite) for  $N_a^2 \rightarrow \infty$ . In such subspaces the Hamiltonian commutes with the  $\eta\nu$  translation generators  $\hat{q}_{\eta\nu x_1}$  and  $\hat{q}_{\eta\nu x_2}$  in the presence of the corresponding fictitious magnetic field  $\vec{B}_{\eta\nu}$  (and  $s1$  translation generators  $\hat{q}_{s1 x_1}$  and  $\hat{q}_{s1 x_2}$  plus  $s\nu$  translation generators  $\hat{q}_{s\nu x_1}$  and  $\hat{q}_{s\nu x_2}$  in the presence of the corresponding fictitious magnetic fields  $\vec{B}_{s1}$  and  $\vec{B}_{s\nu}$ , respectively). In these subspaces the  $N_{\alpha\nu}$   $\alpha\nu \neq s1$  fermions correspond to a zero-momentum and vanishing-energy occupancy and are invariant under the electron - rotated-electron unitary transformation. Indeed, they obey the criterion of Eq. (41). When all  $\alpha\nu \neq s1$  fermions of a given branch have that invariance their number  $N_{\alpha\nu}$  is conserved so that in the present case the numbers  $B_\alpha$  and  $N_{\alpha 1}^h$  where  $\alpha = \eta, s$  and  $N_{s1}$  if  $\alpha = s$  can be expressed solely in terms of good quantum numbers so that they are good quantum numbers as well.

B) In subspaces where  $N_{a\eta\nu}^2 = 2S_\eta$  (and  $N_{a s\nu}^2 = 2S_s$ ) for all branches with  $\nu \geq 1$  (and  $\nu \geq 2$ ) then  $N_{\eta\nu} = 0$  and  $N_{\eta\nu}^h = 2S_\eta$  (and  $N_{s\nu} = 0$  and  $N_{s1}^h = 2S_s$ ) are good quantum numbers for all such branches. In addition,  $B_\eta = 0$  (and  $B_s = [S_c - S_s]$ ,  $N_{a s1}^2 = [S_c + S_s]$ ,  $N_{s1} = [S_c - S_s]$ , and  $N_{s1}^h = 2S_s$ ) are good quantum numbers as well. This follows straightforwardly from  $S_\eta$ ,  $S_s$ , and  $S_c$  being conserved. In such subspaces the Hamiltonian commutes with the  $s1$  translation generators  $\hat{q}_{s1 x_1}$  and  $\hat{q}_{s1 x_2}$  in the presence of the corresponding fictitious magnetic field  $\vec{B}_{s1}$ .

The Hubbard model on a square-lattice in a subspace (A) and or in a subspace (B) provided that  $S_s = 0$  has in the limit  $U/4t \rightarrow \infty$  an interesting physics. For such subspaces the  $\alpha\nu$  fermion occupancy configurations are in that limit and within a mean-field approximation for the fictitious magnetic field  $\vec{B}_{\alpha\nu}$  of Eq. (25) closely related to the physics of a full lowest Landau level of the 2D quantum Hall effect (QHE). Consider for instance a subspace (A) with  $S_s = 0$ ,  $N_{s1}$  and  $N_{s\nu}$  finite where  $\nu \neq 1$ ,  $N_{s\nu'} = 0$  for all remaining  $s\nu'$  branches, and  $2\nu N_{s\nu}/N_a^2/N_a^2 \rightarrow 0$  and  $N_{a s1}^2/N_a^2$  finite for  $N_a^2 \rightarrow \infty$ . From the use of Eqs. (42) and (43) one then finds that  $N_{a s1}^2 = N_{s1}[1 + \mathcal{O}(1/N_a^D)] = N_{s1}$  and  $N_{a s\nu}^2 = N_{s\nu}$  for  $N_a^2 \rightarrow \infty$ . That corresponds to the case when  $\langle n_{\vec{r}_j, s1} \rangle \approx 1$  and  $\langle n_{\vec{r}_j, s\nu} \rangle \approx 1$  and if in the mean field approximation one replaces the corresponding fictitious magnetic fields by the average fields created by all  $s1$  and  $s\nu$  fermions, respectively, at a given position one finds as above  $\vec{B}_{s1}(\vec{r}_j) \approx [\Phi_0/a_{s1}^2] \vec{e}_{x_3}$  and  $\vec{B}_{s\nu}(\vec{r}_j) \approx [\Phi_0/a_{s\nu}^2] \vec{e}_{x_3}$ . The numbers of  $s1$  and  $s\nu$  band discrete momentum values can then be written as,

$$N_{a s1}^2 = \frac{B_{s1} L^2}{\Phi_0}; \quad \nu_{s1} = \frac{N_{s1}}{N_{a s1}^2} = 1; \quad N_{a s\nu}^2 = \frac{B_{s\nu} L^2}{\Phi_0}; \quad \nu_{s\nu} = \frac{N_{s\nu}}{N_{a s\nu}^2} = 1. \quad (66)$$

A similar relation  $N_{a\eta\nu}^2 = B_{\eta\nu} L^2/\Phi_0$  is found for subspaces (A) when there is an occupied  $\eta\nu$  band and for the  $s1$  fermions alone for subspaces (B) and  $S_s = 0$ . It is found in Ref.<sup>1</sup> that the  $\alpha\nu$  fermions have a momentum dependent energy dispersion and only in the limit  $U/4t \rightarrow \infty$  their energy bandwidth vanishes. Hence only in that limit are the  $N_{a s1}^2$  one- $s1$ -fermion states and  $N_{a s\nu}^2$  one- $s\nu$ -fermion states of Eq. (66) degenerate. It follows that in such a limit  $N_{a s1}^2 = B_{s1} L^2/\Phi_0$  and  $N_{a s\nu}^2 = B_{s\nu} L^2/\Phi_0$  play the role of the number of degenerate states in each Landau level of the 2D QHE. In the subspaces considered here the  $\alpha\nu$  fermion occupancies correspond to a full lowest Landau level with filling factor one, as given in Eq. (66). Only for the  $U/4t \rightarrow \infty$  limit there is fully equivalence between the  $\alpha\nu$  fermion occupancy configurations and, within a mean-field approximation for the fictitious magnetic field  $\vec{B}_{\alpha\nu}$  of Eq. (25), the 2D QHE with a  $\nu_{\alpha\nu} = 1$  full lowest Landau level. In spite of the lack of state degeneracy emerging upon decreasing the value of  $U/4t$ , there remains for finite  $U/4t$  values some relation to the 2D QHE. The occurrence of QHE-type behavior in the square-lattice quantum liquid shows that a magnetic field is not essential to the 2D QHE physics. Indeed, here the fictitious magnetic fields arise from expressing the effects of the electronic correlations in terms of the  $\alpha\nu$  fermion interactions.

The mean-field analysis associated with Eq. (66) is consistent with in the subspaces (A) and (B) the square-lattice model Hamiltonian commuting with the  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu}$  in the  $U/4t \rightarrow \infty$  limit so that their eigenvalues are good quantum numbers. Indeed, in that limit such an analysis refers to an effective description where the Hamiltonian is the sum of a  $c$  fermion kinetic-energy term and a QHE like Hamiltonian for each  $\alpha\nu$  branch. The  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu}$  then commute with all such Hamiltonian terms so that in the  $U/4t \rightarrow \infty$  limit their eigenvalues are indeed good quantum numbers for the model on the square lattice in a subspace (A) or (B). Since the electron - rotated-electron transformation is unitary such commutation relations also hold for  $U/4t > 0$  so that in such subspaces the  $\alpha\nu$  fermion discrete momentum values are indeed good quantum numbers for  $U/4t$  finite as well.

In summary, for the Hubbard model on the square lattice each  $U/4t > 0$  energy eigenstate  $|\Psi_{U/4t}\rangle = \hat{V}^\dagger |\Psi_\infty\rangle$  where  $\hat{V}$  is the uniquely defined electron - rotated-electron unitary operator considered in this paper can be expressed as a superposition of a set of  $S_\eta, S_\eta^z, S_s, S_s^z, S_c$ , and momentum eigenstates  $|\Phi_{U/4t}\rangle = \hat{V}^\dagger |\Phi_\infty\rangle$  of general form given in Eq. (61) with equal values for such physical quantities,  $c$  fermion momentum distribution function  $N_c(\vec{q}) = N_{rot}(\vec{q})$  of Eq. (65), and numbers  $C_\alpha = \sum_{\nu=1}^{C_\alpha} \nu N_{\alpha\nu}$  of Eqs. (20), (21), (31), and (47) where  $\alpha = \eta, s$  but different values for the  $\alpha\nu$  fermion numbers  $\{N_{\alpha\nu}\}$ . However, in some limiting cases such as for the energy eigenstates that span the one- and two-electron subspace that set reduces to a single state  $|\Phi_{U/4t}\rangle$  so that  $|\Psi_{U/4t}\rangle = |\Phi_{U/4t}\rangle$ . In turn, that for the 1D model the whole set of  $\alpha\nu$  fermion numbers  $\{N_{\alpha\nu}\}$  are good quantum numbers and the corresponding  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu}$  commute with the Hamiltonian is behind the equality  $|\Psi_{U/4t}\rangle = |\Phi_{U/4t}\rangle$  always holding.

#### F. Number of $s1$ fermion holes of the elementary excitations of $x > 0$ and $m = 0$ ground states

The number  $N_{s1}^h$  of unoccupied sites of the  $s1$  effective lattice equals that of  $s1$  fermion holes in the  $s1$  momentum band and plays an important role in the general energy spectrum of the square-lattice quantum liquid introduced in this paper and further studied in Refs.<sup>1,22</sup>. Indeed, for the one- and two-electron subspace it is a good quantum number. Here we address the problem of the  $N_{s1}^h$  expression in terms of the number  $N$  of electrons, which contains important physical information. For the index choice  $\alpha = s$ , Eq. (44) reads  $N_{s1}^h = [N_{a_s}^D - 2B_s]$  where  $N_{a_s}^D = 2S_c$  is the number of sites of the spin effective lattice and  $B_s$  the number defined in Eqs. (44) and (47). From the use of expression  $a_\alpha = L/N_{a_\alpha} = [N_a/N_{a_\alpha}]a$  given in Eq. (30) where  $\alpha = \eta, s$ , the number of unoccupied sites of the  $s1$  effective lattice can be rewritten as  $N_{s1}^h = [N_a^D - N_{a_\eta}^D - 2B_s]$  where  $N_{a_\eta}^D = [N_a^D - 2S_c]$  is the number of sites of the  $\eta$ -spin effective lattice. From combination of the expressions given in Eqs. (19) and (22) one finds  $N_{a_\eta}^D = [N_a^D - N + 2C_\eta + 2L_{\eta,-1/2}]$  where  $C_\eta$  is given in Eq. (31) and  $L_{\eta,-1/2}$  is the number of independent  $-1/2$   $\eta$ -spinons. The use of that result in the above general  $N_{s1}^h$  expression leads to,

$$N_{s1}^h = [N - 2B_s - 2C_\eta - 2L_{\eta,-1/2}]. \quad (67)$$

For the model on the square lattice this number labels the momentum eigenstates of Eq. (61) but in general is not a good quantum number because the number  $B_s$  on the right-hand side of Eq. (67) given in Eqs. (44) and (47) is not in general conserved. (All remaining numbers on its right-hand side are.)

Since all sites of the  $s1$  effective lattice of  $x > 0$  and  $m = 0$  ground states are occupied and hence there are no unoccupied sites, from the use of such a  $N_{s1}^h$  expression one finds that for the corresponding excited states the number of unoccupied sites of the  $s1$  effective lattice and thus of  $s1$  fermion holes in the  $s1$  momentum band reads,

$$\begin{aligned} N_{s1}^h &= [\delta N - 2\delta N_{s1} - 2 \sum_{\nu=2}^{C_s} N_{s\nu} - 2C_\eta - 2L_{\eta,-1/2}] \quad (\text{general}), \\ N_{s1}^h &= [\delta N - 2\delta N_{s1} - 2N_{s2}] \quad (\text{one- and two- electron subspace}). \end{aligned} \quad (68)$$

Here  $\delta N$  and  $\delta N_{s1}$  are the electron and  $s1$  fermion number deviations, respectively, generated in the transitions from the above ground states to the excited states. Since  $x > 0$  and  $m = 0$  ground states have no  $2\nu$ -spinon composite  $s\nu$  fermions with  $\nu \geq 2$  spinon pairs, no  $2\nu$ - $\eta$ -spinon composite  $\eta\nu$  fermions, and no independent  $-1/2$   $\eta$ -spinons, the deviations in the corresponding numbers  $N_{s\nu}$ ,  $C_\eta = \sum_{\nu=1}^{C_\eta} \nu N_{\eta\nu}$ , and  $L_{\eta,-1/2}$  equal the corresponding excited-state numbers. The expressions given in Eq. (68) refer to the latter numbers.

The first expression is valid for the whole Hilbert space of the Hubbard model and hence takes into account all available excited states. It reveals that the number of holes in the  $s1$  momentum band can be written as  $N_{s1}^h = \delta[N - N_{s1}^{\delta N}]$  where the absolute value of the number  $N_{s1}^{\delta N} \equiv [\delta N - N_{s1}^h]$  given in Eq. (68) is always an even number. Therefore, for  $\delta N = \pm 1$  one-electron excited states  $N_{s1}^h$  must be always an odd integer. In turn, for  $\delta N = 0$  and  $\delta N = \pm 2$  two-electron excited states  $N_{s1}^h$  must be always an even integer. Hence one-electron (and two-electron) excitations do not couple to excited states with two holes (and a single hole) in the  $s1$  momentum band.



The second expression provided in Eq. (68) refers to the one- and two-electron subspace defined in the ensuing section. The states that span such a subspace are of type (A) or (B) so that for them all numbers involved in that expression are good quantum numbers for the model on the square lattice, as confirmed below.

## V. THE SQUARE-LATTICE QUANTUM LIQUID: A TWO-COMPONENT FLUID OF CHARGE $c$ FERMIONS AND SPIN-NEUTRAL TWO-SPINON $s1$ FERMIONS

In this section we introduce and define the one- and two-electron subspace and corresponding spin and  $s1$  effective lattices, whereas the  $c$  and  $s1$  momentum bands associated with the  $c$  and  $s1$  effective lattices, respectively, are studied in Ref.<sup>1</sup>. Moreover, here we address the problem of the generation of the one- and two-electron spectral weight in terms of processes of  $c$  fermions and spinons. The picture which emerges is that of a two-component quantum liquid of charge  $c$  fermions and spin neutral two-spinon  $s1$  fermions. For the model on the square lattice it refers to the square-lattice quantum liquid further studied in Refs.<sup>1,22</sup>.

### A. The one- and two-electron subspace as defined in this paper

Let  $|\Psi_{GS}\rangle$  be the exact ground state for  $x \geq 0$  and  $m = 0$  and  $\hat{O}$  denote an one- or two-electron operator. Then the state,

$$\hat{O}|\Psi_{GS}\rangle = \sum_j C_j |\Psi_j\rangle; \quad C_j = \langle \Psi_j | \hat{O} | \Psi_{GS} \rangle, \quad (69)$$

generated by application of  $\hat{O}$  onto that ground state is contained in the general one- and two-electron subspace. This is the subspace spanned by the set of energy eigenstates  $|\Psi_j\rangle$  such that the corresponding coefficients  $C_j$  are not vanishing.

Our goal is finding a set of excited states that have nearly the whole spectral weight  $\sum_j |C_j|^2 \approx 1$  of the above one- and two-electron excitations. For a  $x > 0$  (and  $x = 0$ ) and  $m = 0$  ground state  $|\Psi_{GS}\rangle$  it is found here that such states have excitation energy  $\omega < 2\mu$  (and  $\omega < \mu^0$ ). The inequality  $\omega < 2\mu$  applies to hole concentrations  $0 < x < 1$  and  $m = 0$ . In turn, for the  $\mu = 0$  and  $m = 0$  absolute ground state with the chemical-potential zero level at the middle of the Mott-Hubbard gap the smallest energy required for creation of both one rotated-electron and one rotated-hole doubly occupied site is instead given by the energy scale  $\mu^0$ . This justifies why for such initial ground state the above inequality  $\omega < 2\mu$  is replaced by  $\omega < \mu^0$ .

From the use of the invariance under the electron - rotated-electron unitary transformation of the independent  $\pm 1/2$  spinons, one finds that the number of such objects generated by application of  $\mathcal{N}$ -electron operators onto a ground state is exactly restricted to the following range,

$$L_s = [L_{s,-1/2} + L_{s,+1/2}] = 2S_s = 0, 1, 2, \dots, \mathcal{N}. \quad (70)$$

It follows that for the one- and two-electron subspace only the values  $L_s = [L_{s,-1/2} + L_{s,+1/2}] = 2S_s = 0, 1, 2$  are allowed. Such a restriction is exact for both the model on the square and 1D lattices.

An important property is that for a number  $\nu \geq 2$  of spinon pairs the  $s\nu$  fermions created onto a  $x \geq 0$  and  $m = 0$  ground state have vanishing energy and momentum. Since at  $m = 0$  one has that  $H = 0$ , such objects obey the criterion  $\epsilon_{s\nu} = 2\nu\mu_B H = 0$  of Eq. (41). Hence they are invariant under the electron - rotated-electron unitary transformation. Therefore, for  $U/4t > 0$  they correspond to the same occupancy configurations in terms of both rotated electrons and electrons. That reveals that such  $s\nu$  fermions describe the spin degrees of freedom of a number  $2\nu$  of electrons. It follows that nearly the whole spectral weight generated by application onto the ground state of  $\mathcal{N}$ -electron operators refers to a subspace spanned by energy eigenstates with numbers in the following range,

$$[L_{s,-1/2} + L_{s,+1/2} + 2C_s - 2B_s] = 0, 1, 2, \dots, \mathcal{N}. \quad (71)$$

Note that owing to the above invariance of the  $s\nu$  fermions with  $\nu \geq 2$  spinon pairs under consideration provided that  $\mathcal{N}/N_a^D \rightarrow 0$  and  $B_s/N_a^D \rightarrow 0$  for  $N_a^D \rightarrow \infty$  the number  $B_s = \sum_\nu N_{s\nu}$  is a good quantum number. (This is a generalization of the subspace (A) considered in Subsection IV-D.) Consistently, the  $x > 0$  (and  $x = 0$  and  $\mu = 0$ ) and  $m = 0$  ground state and the set of excited states of energy  $\omega < 2\mu$  (and  $\omega < \mu^0$ ) that span the one- and two-electron subspace introduced in this paper have no  $-1/2$   $\eta$ -spinons,  $\eta\nu$  fermions, and  $s\nu'$  fermions with  $\nu' \geq 3$  spinon pairs so that  $N_{\eta\nu} = 0$  and  $N_{s\nu'} = 0$  for  $\nu' \geq 3$ . As further discussed below, summation over the states that span that subspace as defined here gives  $\sum_j |C_j|^2 \approx 1$  for the coefficients of the one- or two-electron excitation  $\hat{O}|\Psi_{GS}\rangle$  of Eq. (69) and

numbers	charge	+1↑el.	-1↓el.	+1↓el.	-1↑el.	singl.spin	tripl.spin	tripl.spin	tripl.spin	±2↑↓el.	+2↑el.	-2↓el.	+2↓el.	-2↑el.
$\delta N_c^h$	0	-1	1	-1	1	0	0	0	0	±2	-2	2	-2	2
$N_{s1}^h$	0	1	1	1	1	2	2	2	2	0	2	2	2	2
$\delta N_\uparrow$	0	1	0	0	-1	0	1	-1	0	±1	2	0	0	-2
$\delta N_\downarrow$	0	0	-1	1	0	0	-1	1	0	±1	0	-2	2	0
$L_{s,+1/2}$	0	1	1	0	0	0	2	0	1	0	2	2	0	0
$L_{s,-1/2}$	0	0	0	1	1	0	0	2	1	0	0	0	2	2
$N_{s2}$	0	0	0	0	0	1	0	0	0	0	0	0	0	0
$S_s$	0	1/2	1/2	1/2	1/2	0	1	1	1	0	1	1	1	1
$\delta S_c$	0	1/2	-1/2	1/2	-1/2	0	0	0	0	±1	1	-1	1	-1
$\delta N_{s1}$	0	0	-1	0	-1	-2	-1	-1	-1	±1	0	-2	0	-2
$\delta N_{a_{s1}}$	0	1	0	1	0	0	1	1	1	±1	2	0	2	0

TABLE I: The deviations  $\delta N_c^h = -2\delta S_c$  and numbers  $N_{s1}^h = [2S_s + 2N_{s2}]$  of Eq. (73) for the fourteen classes of one- and two-electron excited states of the  $x > 0$  and  $m = 0$  ground state that span the one- and two-electron subspace as defined in this paper and Ref.<sup>1</sup>, corresponding electron number deviations  $\delta N_\uparrow$  and  $\delta N_\downarrow$ , and independent-spinon numbers  $L_{s,+1/2}$  and  $L_{s,-1/2}$  and  $s2$  fermion numbers  $N_{s2}$  restricted to the values provided in Eq. (72). The spin  $S_s$  and deviations  $\delta S_c$ ,  $\delta N_{s1} = [\delta S_c - S_s - 2N_{s2}]$ , and  $\delta N_{a_{s1}} = [\delta S_c + S_s]$  of each excitation are also provided.

there is both for the model on the 1D and square lattices an extremely small weight corresponding mostly to states with  $N_{s3} = 1$ , which is neglected within our definition of the one- and two-electron subspace.

Thus, according to Eq. (71) the numbers of independent  $\pm 1/2$  spinons and that of  $s2$  fermions of the excited states that span such a subspace are restricted to the following ranges,

$$\begin{aligned} L_{s,\pm 1/2} &= 0, 1; \quad N_{s2} = 0, \quad \text{for } \mathcal{N} = 1, \\ 2S_s + 2N_{s2} &= [L_{s,-1/2} + L_{s,+1/2} + 2N_{s2}] = 0, 1, 2, \quad \text{for } \mathcal{N} = 2. \end{aligned} \quad (72)$$

Here  $\mathcal{N} = 1, 2$  refers to the  $\mathcal{N}$ -electron operators  $\hat{O}$  whose application onto the ground state  $|\Psi_{GS}\rangle$  generates the above excited states, as given in Eq. (69). Furthermore,  $N_c = N = (1-x)N_a^D$  and  $N_{s1} = [N/2 - 2N_{s2} - S_s] = (1-x)N_a^D/2 - [2N_{s2} + S_s]$ . If in addition we restrict our considerations to the LWS-subspace of the one- and two-electron subspace, then  $L_{s,-1/2} = 0$  in Eq. (72), whereas the values  $L_{s,+1/2} = 0, 1$  for  $N_{s2} = 0$  and  $\mathcal{N} = 1$  remain valid and in  $[2S_s + 2N_{s2}] = 0, 1, 2$  one has that  $2S_s = L_{s,+1/2}$  for  $\mathcal{N} = 2$ .

We recall that the numbers of independent  $\eta$ -spinons ( $\alpha = \eta$ ) and independent spinons ( $\alpha = s$ )  $L_{\alpha,\pm 1/2}$ , total numbers of  $\eta$ -spinons ( $\alpha = \eta$ ) and spinons ( $\alpha = s$ )  $M_{\alpha,\pm 1/2} = [L_{\alpha,\pm 1/2} + C_\alpha]$ , number of sites of the spin effective lattice  $N_{a_s}^D = 2S_c$ , number of sites of the  $\eta$ -spin effective lattice  $N_{a_\eta}^D = [N_a^D - 2S_c]$ , number of  $c$  fermions  $N_c = 2S_c$ , and number of  $c$  fermion holes  $N_c^h = [N_a^D - 2S_c]$  are good quantum numbers of both the Hubbard model on the 1D and square lattices. The good news is that in the one- and two-electron subspace as defined here the numbers  $N_{a_{s1}}^2$ ,  $N_{s1}$ ,  $N_{s1}^h$ , and  $N_{s2}$  are good quantum numbers of the Hubbard model on the square lattice as well. Indeed, for spin  $S_s = 0$  that subspace is a subspace (A) as defined in Subsection IV-D so that  $N_{s1} = [S_c - 2N_{s2}]$ ,  $N_{s1}^h = 2N_{s2}$ , and  $N_{s2}$  and hence  $N_{a_{s1}}^2 = [N_{s1} + N_{s1}^h] = S_c$  are good quantum numbers. Furthermore, for the remaining spin values  $S_s = 1/2$  and  $S_s = 1$  such a subspace is a subspace (B) as defined in that subsection so that  $N_{s1} = [S_c - S_s]$ ,  $N_{s1}^h = 2S_s$ , and  $N_{a_{s1}}^2 = [S_c + S_s]$  are good quantum numbers. That implies that the microscopic momenta  $\vec{q}$  carried by the  $s1$  fermions are good quantum numbers.

The number of sites, unoccupied sites, and occupied sites of the  $c$  and  $s1$  effective lattices equal those of discrete momentum values, unfilled momentum values, and filled momentum values of the  $c$  and  $s1$  bands, respectively. Use of the general expressions of  $s1$  band discrete momentum values and number  $N_{s1}^h$  of  $s1$  band unfilled momentum values given in Eq. (44) for  $\alpha = s$  together with the restrictions in the values of the numbers of Eqs. (70), (71), and (72) and the result proved above in Subsection IV-E that one-electron (and two-electron) excitations have no overlap with excited states with none and two (and one)  $s1$  band holes (and hole) reveals that nearly the whole one- and two-electron spectral weight is contained in the subspace spanned by states whose deviation  $\delta N_c^h$  in the number of  $c$  band holes and number  $N_{s1}^h$  of  $s1$  band holes are given by,

$$\begin{aligned} \delta N_c^h &= -2\delta S_c = -\delta N = 0, \mp 1, \mp 2, \\ N_{s1}^h &= 2S_s + 2N_{s2} = \pm(\delta N_\uparrow - \delta N_\downarrow) + 2L_{s,\mp 1/2} + 2N_{s2} = L_{s,-1/2} + L_{s,+1/2} + 2N_{s2} = 0, 1, 2. \end{aligned} \quad (73)$$

Here  $\delta N$  is the deviation in the number of electrons,  $\delta N_\uparrow$  and  $\delta N_\downarrow$  those in the number of spin-projection  $\uparrow$  and  $\downarrow$  electrons, respectively,  $N_{s2}$  the number of the excited-state  $s2$  fermions, and  $L_{s,\pm 1/2}$  that of independent spinons of spin projection  $\pm 1/2$ . The deviations  $\delta N_c^h$  and numbers  $N_{s1}^h$  of Eq. (73) for the fourteen classes of one- and

two-electron excited states of the  $x > 0$  and  $m = 0$  ground state that span the one- and two-electron subspace, corresponding electron number deviations  $\delta N_\uparrow$  and  $\delta N_\downarrow$ , and independent-spinon numbers  $L_{s,+1/2}$  and  $L_{s,-1/2}$  and  $s_2$  fermion numbers  $N_{s_2}$  restricted to the values provided in Eq. (72) are given in Table I. For excited states with  $N_{s_2} = 1$  the  $s_2$  effective lattice has a single site and the corresponding  $s_2$  band a single vanishing discrete momentum value,  $\vec{q} = 0$ , occupied by the  $s_2$  fermion. Such a  $s_2$  fermion is invariant under the electron - rotated-electron unitary transformation and has zero energy, consistently with the invariance condition of Eq. (41) for  $\alpha\nu = s_2$  and zero magnetic field  $H = 0$ .

The initial  $x > 0$  and  $m = 0$  ground states of the one- and two-electron subspace have zero holes in the  $s_1$  band so that  $\delta N_{s_1}^h = N_{s_1}^h$  for the excited states. The one- and two-electron subspace as defined here is spanned by the states of Table I generated by creation or annihilation of  $|\delta N_c^h| = 0, 1, 2$  holes in the  $c$  momentum band and  $N_{s_1}^h = 0, 1, 2$  holes in the  $s_1$  band plus small momentum and low energy particle-hole processes in the  $c$  band. The charge excitations of  $x > 0$  and  $m = 0$  initial ground states consist of a single particle-hole process in the  $c$  band of arbitrary momentum and energy compatible with its momentum and energy bandwidths, plus small-momentum and low-energy  $c$  fermion particle-hole processes. Such charge excitations correspond to state representations of the global  $U(1)$  symmetry and refer to the type of states denoted by "charge" in the table. The one-electron spin-doublet excitations correspond to the four types of states denoted by " $\pm 1\sigma_{el}$ ." in Table I where  $+1$  and  $-1$  denotes creation and annihilation, respectively, and  $\sigma = \uparrow, \downarrow$ . The spin-singlet and spin-triplet excitations refer to the four types of states denoted by "singl.spin" and "tripl.spin" in the table. The two-electron excitations whose electrons are in a spin-singlet configuration and those whose two created or annihilated electrons are in a spin-triplet configuration correspond to the five types of states " $\pm 2\uparrow\downarrow_{el}$ ." and " $\pm 2\sigma_{el}$ ." of that table where  $+2$  and  $-2$  denotes creation and annihilation, respectively, of two electrons.

Alike for the 1D model, for the model on the square lattice such fourteen types of states are energy eigenstates and contain nearly the whole one- and two-electron spectral weight. Excited states of classes other than those of the table contain nearly no one- and two-electron spectral weight. Such a weight analysis applies to the 1D Hubbard model as well. Moreover, for the quantum liquid corresponding to the Hamiltonian (1) in the one- and two-electron subspace as defined in this paper, the numbers  $2S_c$ ,  $2S_\eta$ ,  $2S_s$ , and  $-2S_s^z$  associated with the global  $SO(3) \times SO(3) \times U(1)$  symmetry are given by,

$$2S_c = (1-x) N_a^D; \quad 2S_\eta = -2S_\eta^z = x N_a^D; \quad 2S_s = (1-x) N_a^D - 2[N_{s_1} + 2N_{s_2}]; \quad -2S_s^z = m N_a^D = 2S_s - 2L_{s,-1/2}. \quad (74)$$

For such a quantum liquid the number of sites and lattice spacing of the spin effective lattice read,

$$N_{a_s}^D = (1-x) N_a^D; \quad a_s = \frac{a}{(1-x)^{1/D}}, \quad (1-x) \geq 1/N_a^D. \quad (75)$$

We emphasize that for the model in the one- and two-electron subspace the concept of a  $\eta$ -spin lattice has no physical significance because the  $\eta$ -spin degrees of freedom refer to the  $C_\eta = (N_a^D/2 - S_c - S_\eta) = 0$  vacuum  $|0_\eta; N_{a_\eta}^D\rangle$  of Eq. (23), which for  $S_c > 0$  corresponds to a single occupancy configuration of the  $N_{a_\eta}^D + 1/2$   $\eta$ -spinons. Only when both  $N_{a_\eta}^D/N_a^D = [1 - 2S_c/N_a^D] > 0$  and  $C_\eta = (N_a^D/2 - S_c - S_\eta) > 0$  is the concept of a  $\eta$ -spin effective lattice well defined and useful. Indeed, for that subspace the numbers  $C_\eta$  and  $C_s$  of sites of the original lattice whose electron occupancy configurations that generate the energy and momentum eigenstates are not invariant under the electron - rotated-electron unitary transformation are given by  $C_\eta = 0$  and  $C_s = [N_{s_1} + 2N_{s_2}]$ , respectively. For  $x = 0$  (and  $x = 1$ ) one finds  $N_{a_\eta}^D = 0$  and  $N_{a_s}^D = N_a^D$  (and  $N_{a_\eta}^D = N_a^D$  and  $N_{a_s}^D = 0$ ), so that there is no  $\eta$ -spin (and no spin) effective lattice and the spin (and  $\eta$ -spin) effective lattice equals the original lattice.

As further confirmed below in Subsection V-D, for the one- and two-electron subspace defined here only the  $c$  and  $s_1$  fermions have an active role. Straightforward manipulations of the above general expressions given in Eqs. (42)-(53) reveal that for that subspace the number  $N_{a_{s_1}}^D$  of  $s_1$  band discrete momentum values,  $N_{s_1}$  of  $s_1$  fermions, and  $N_{s_1}^h$  of  $s_1$  fermion holes are given by,

$$N_{a_{s_1}}^D = [N_{s_1} + N_{s_1}^h] = [S_c + S_s]; \quad N_{s_1} = [S_c - S_s - 2N_{s_2}]; \quad N_{s_1}^h = [2S_s + 2N_{s_2}] = 0, 1, 2, \quad (76)$$

respectively. In turn, the corresponding  $c$  effective lattice,  $c$  momentum band, and  $c$  fermion numbers read,

$$N_{a_c}^D = [N_c + N_c^h] = N_a^D; \quad N_c = 2S_c = (1-x) N_a^D; \quad N_c^h = x N_a^D. \quad (77)$$

As mentioned above, for states belonging to the one- and two-electron subspace the  $\eta$ -spin degrees of freedom correspond to a single occupancy configuration referring to the  $\eta$ -spin vacuum  $|0_\eta; N_{a_\eta}^D\rangle$  of Eq. (23) (and to no configuration since  $N_{a_\eta}^D = 0$  in that vacuum). Therefore, when defined in that subspace the Hamiltonian (1) has an effective global  $U(2)/Z_2 \equiv SO(3) \times U(1)$  symmetry. This is anyway the global symmetry relevant to more general models belonging to the same universality class as that considered here. Indeed, the  $\eta$ -spin  $SU(2)$  symmetry disappears if one adds to the Hamiltonian (1) kinetic-energy terms involving electron hopping beyond nearest neighbors. In contrast, the global  $SO(3) \times U(1)$  symmetry is robust under the addition of such terms.

### B. Generation of the one- and two-electron spectral weight in terms of processes of $c$ fermions and spinons

Expression by use of the operator relations given in Eq. (17) of the operator  $\tilde{O}$  corresponding to the one- and two-electron operators of the excitations  $\hat{O}|\Psi_{GS}\rangle$  of Eq. (69) in terms of the of  $c$  fermion and rotated quasi-spin operators reveals that the elementary processes associated with the number value ranges of Eqs. (71), (72), and (73) are for the one- and two-electron subspace fully generated by the operator  $\tilde{O}$ .

In turn, expressing by means of the operator relations provided in Eq. (17) the operator terms of Eq. (3) containing commutators involving the operator  $\tilde{S} = (t/U)[\tilde{T}_{+1} - \tilde{T}_{-1}] + \mathcal{O}(t^2/U^2)$  in terms of the of  $c$  fermion and rotated quasi-spin operators and taking into account that independently of their form, the additional operator terms  $\mathcal{O}(t^2/U^2)$  of higher order are products of the kinetic operators  $\tilde{T}_0$ ,  $\tilde{T}_{+1}$ , and  $\tilde{T}_{-1}$  of Eq. (2), one finds that the processes generated by such operator terms refer only to excitations whose number value ranges are different from those of Eqs. (71), (72), and (73) for the one- and two-electron subspace. That confirms that such processes generate very little one- and two-electron spectral weight, consistently with the discussions and analysis of Subsections II-A and V-A.

For the model on the 1D lattice the spectral-weight distributions can be calculated explicitly by the pseudofermion dynamical theory associated with the model exact solution, exact diagonalization of small chains, and other methods. The relative one-electron spectral weight generated by different types of microscopic processes is studied by means of such methods in Ref.<sup>47</sup>. The results of that reference confirm the dominance of the processes associated with the number value ranges provided in Eqs. (72) and (73). In this case the general operators  $\hat{O}$  and  $\tilde{O}$  are electron and rotated-electron, respectively, creation or annihilation operators. The operator  $\tilde{O}$  generates *all* processes associated with the number value ranges of Eqs. (72) and (73) and number values of Table I. In addition, it also generates some of the non-dominant processes. That is confirmed by the weights given in Table 1 of Ref.<sup>47</sup>, which correspond to the dominant processes associated with only these ranges. The small missing weight refers to excitations whose number value ranges are not those of Eqs. (72) and (73) but whose weight is also generated by the operator  $\tilde{O}$ . Indeed, that table refers to  $U/4t \rightarrow \infty$  so that  $\hat{O} = \tilde{O}$  and the operator terms of Eq. (3) containing commutators involving the operator  $\tilde{S}$  vanish because all such commutators vanish in that limit.

On the other hand, for finite values of  $U/4t$  all dominant processes associated with the number value ranges of Eqs. (72) and (73) and number values provided in Table I are generated by the operator  $\tilde{O}$  whereas the small spectral weight associated with excitations whose number value ranges are different from those are generated both by that operator and the operator terms of Eq. (3) containing commutators involving the operator  $\tilde{S}$ . For the model on the 1D lattice the small one-electron spectral weight generated by the non-dominant processes is largest at half filling and  $U/4t \approx 1$ . For the range of hole concentrations  $x \geq 0$  considered in this paper the one- and two-electron subspace is spanned by states with vanishing rotated-electron double occupancy. Its generalization for the range  $x \leq 0$  reveals that then it is spanned by states with vanishing rotated-hole double occupancy. That property combined with the particle-hole symmetry explicit at  $x = 0$  and  $\mu = 0$ , implies that the relative spectral-weight contributions from different types of excitations given in Fig. 2 of Ref.<sup>47</sup> for half-filling one-electron addition leads to similar corresponding relative weights for half-filling one-electron removal. Analysis of that figure confirms that for the corresponding one-electron removal spectrum the dominant processes associated with the number value ranges of Eqs. (72) and (73) and number values given in Table I refer to the states called in the figure 1 holon - 1  $s1$  hole states, whose minimum relative weight of about 0.95 is reached at  $U/4t \approx 1$ . For other hole concentrations  $x > 0$  and values of  $U/4t$  the relative weight of such states is always larger than 0.95, as confirmed from analysis of Figs. 1 and 2 and Table 1 of Ref.<sup>47</sup>.

For the Hubbard model on the square lattice the explicit derivation of one- and two-electron spectral weights is a more involved problem. The number value ranges of Eqs. (71), (72), and (73) and number values provided in Table I for the one- and two-electron subspace also apply, implying similar results for the relative spectral weights of one- and two-electron excitations. Furthermore and as discussed above, analysis of expression (68) reveals that for  $\delta N = \pm 1$  (and  $\delta N = \pm 0$  and  $\delta N = \pm 2$ ) excited states the number  $N_{s1}^h$  of holes in the  $s1$  band must be always an odd (and even) integer so that one-electron (and two-electron) excitations do not couple to excited states with two holes (and one hole) in the  $s1$  band. Both such selection rules hold also for the one- and two-electron subspace for which  $N_{s1}^h = [\delta N - 2\delta N_{s1} - 2N_{s2}]$ , as given in Eq. (68).

### C. The spin and $s1$ effective lattices for the one- and two-electron subspace

Within the operator description introduced in this paper, the subspace with relevance for the one- and two-electron physics is the one- and two-electron subspace as defined above, which is spanned by states with no  $\eta\nu$  fermions and no  $s\nu$  fermions with a number  $\nu \geq 3$  of spinon pairs. According to the restrictions and numbers values of Eqs. (72) and (73) and Table I, such states may involve none or one  $s2$  fermion. As confirmed in Refs.<sup>1,22,32</sup>, it is convenient to express the one- and two-electron excitation spectrum relative to initial  $x > 0$  and  $m = 0$  ground states in terms of the

deviations in the numbers of  $c$  effective lattice and  $s1$  effective lattice unoccupied sites given explicitly in Eq. (73) and Table I. Note that the number of  $s1$  fermions provided in Eq. (76) can be written as  $N_{s1} = [(1-x)N_a^D/2 - S_s - 2N_{s2}]$  where  $S_s = 0$  for  $N_{s2} = 1$  and  $S_s = 0, 1/2, 1$  for  $N_{s2} = 0$ . The square-lattice quantum liquid associated with the Hubbard model on the square lattice in the one- and two-electron subspace is further studied in Refs.<sup>1,18</sup>. The studies of Ref.<sup>22</sup> refer to the same quantum liquid perturbed by small 3D anisotropy associated with weak plane coupling.

Since for  $N_{s2} = 1$  states the  $s2$  fermion has vanishing energy and momentum and in addition consistently with Eq. (41) for vanishing magnetic field  $H = 0$  is invariant under the unitary transformation associated with the operator  $\hat{V}$ , the only effect of its creation and annihilation is on the numbers of occupied and unoccupied sites of the  $s1$  effective lattice and thus in the occupancies of the discrete momentum values of the  $s1$  band, as discussed below. Therefore, for the study of the Hamiltonian (1) in the one- and two-electron subspace the only composite object whose internal occupancy configurations in the spin effective lattice are important for the physics is the two-spinon  $s1$  fermion and associated  $s1$  bond particle studied in Ref.<sup>18</sup>.

It is found below in Subsection V-D that for the model in the one- and two-electron subspace as defined in Subsection V-A the presence of independent  $+1/2$  spinons or a composite  $s2$  fermion is felt through the numbers of occupied and unoccupied sites of the  $s1$  effective lattice, whereas the number of independent  $+1/2$   $\eta$ -spinons equals that of the unoccupied sites of the  $c$  effective lattice. Therefore, when acting onto that subspace, the Hubbard model refers to a two-component quantum liquid described in terms of  $c$  fermions and  $s1$  fermions.

For  $N_a^D \gg 1$  the description introduced in Ref.<sup>18</sup> of both the spinon occupancy configurations of a  $s1$  bond-particle associated with a local  $s1$  fermion and of the underlying  $s1$  effective lattice is a good approximation provided that the ratio  $N_{as}^D/N_a$  is finite. Since the number of sites of the spin effective lattice is given by  $N_{as}^D = (1-x)N_a^D$ , that requirement is met provided that the electronic density  $n = (1-x)$  is finite. Such a description is exact for hole concentrations  $0 \leq x \ll 1$  when the spin-effective lattice becomes the original lattice. In that limit all sites of the spin effective lattice become sites of the original square or 1D lattice. In turn, for the model on the square lattice it does not apply when  $x \approx 1$  and there is a finite number of sites in the spin effective lattice only. So it is a good approximation for the range  $(1-x) \geq 1/N_a^D$  and the limit  $N_a^D \gg 1$  considered in our studies. Particularly, it is a good approximation for hole concentrations  $x \in (0, x_*)$  considered in Refs.<sup>1,22</sup>, where  $x_* \in (0.23, 0.28)$  for the range  $U/4t \in (u_0, u_1)$  of interest for the studies of these references where  $u_0 \approx 1.3$  and  $u_1 \approx 1.6$ , respectively.

For  $x < 1$  the spin effective lattice has a number of sites  $N_{as}^D = (1-x)N_a^D$  smaller than that of the original lattice. Nevertheless for  $N_a^D \gg 1$  a site of the spin effective lattice with real-space coordinate  $\vec{r}_j$  in that lattice has a well-defined position  $\vec{r} = \vec{r}_j$  in the original real space contained within the system area or length  $L^D$  where  $D = 2$  and  $D = 1$ , respectively. This is consistent with the lattice constant  $a_s$  defined in Eq. (30) for  $\alpha = s$ , which for the one- and two-electron subspace reads,

$$a_s = \frac{a}{(1-x)^{1/D}}; \quad x \ll 1, \quad D = 1, 2, \quad (78)$$

being such that the area ( $D = 2$ ) or length ( $D = 1$ )  $L^D$  of the system is preserved. Obviously, any real-space point within the spin effective lattice corresponds to the same real-space point in the system original lattice. So the real-space coordinates  $\vec{r}_{j'}$  of the  $j' = 1, \dots, N_{as}^D$  sites of the spin effective lattice are for  $x > 0$  different from the real-space coordinates  $\vec{r}_j$  of the  $j = 1, \dots, N_a^D$  sites of the original lattice. The vectors  $\vec{r}_j$  and  $\vec{r}_{j'}$  refer though to well-defined positions in the same 1D or 2D real space contained within such a lattice.

The suitability of the description introduced in this paper in terms of occupancies of effective lattices is confirmed for 1D by the results of Appendix B: The discrete momentum values of the  $c$  fermions and  $\alpha\nu$  fermions correspond to quantum numbers of the model exact solution. In turn, no exact solution exists for the model on the square lattice. However, the discrete momentum values obtained for such objects refer to good quantum numbers for that model in the one- and two-electron subspace.

For such a  $N_a^D \gg 1$  subspace there is commensurability between the real-space distributions of the  $N_{as1}^D \approx N_{s1}$  sites of the  $s1$  effective lattice and the  $N_{as}^D \approx 2N_{s1}$  sites of the spin effective lattice. For  $(1-x) \geq 1/N_a^D$  and  $N_a^D \gg 1$  the spin effective lattice has  $N_{as}^D = (1-x)N_a^D$  sites and from the use of the expression given in Eq. (76) for  $N_{as1}^D$  and Eq. (53) for  $a_{s1}$  we find,

$$a_{s1} = 2^{1/D} a_s \frac{1}{\left(1 + \frac{2S_s}{(1-x)N_a^D}\right)^{1/D}} \approx 2^{1/D} a_s \left(1 - \frac{2S_s}{D(1-x)N_a^D}\right) \approx 2^{1/D} a_s, \quad 2S_s = 0, 1, 2. \quad (79)$$

For  $N_{s1}^h = 0$  states the bipartite 1D and square spin effective lattices have two well-defined sub-lattices. As discussed in Ref.<sup>18</sup>, for  $N_{s1}^h = 1, 2$  states the spin effective lattice has two bipartite lattices as well, with one or two extra sites corresponding to suitable boundary conditions. For the model on the square lattice the two spin effective sub-lattices have lattice constant  $a_{s1} = \sqrt{2}a_s$ . In turn, for 1D the sites of each spin effective sub-lattice are

distributed alternately along the chain, the corresponding nearest-neighboring sites being separated by  $a_{s1} = 2a_s$ . The fundamental translation vectors of such sub-lattices read,

$$\vec{a}_{s1} = a_{s1} \vec{e}_{x_1} \text{ for } 1D; \quad \vec{a}_{s1} = \frac{a_{s1}}{\sqrt{2}}(\vec{e}_{x_1} + \vec{e}_{x_2}), \quad \vec{b}_{s1} = -\frac{a_{s1}}{\sqrt{2}}(\vec{e}_{x_1} - \vec{e}_{x_2}) \text{ for } 2D, \quad (80)$$

where  $\vec{e}_{x_1}$  and  $\vec{e}_{x_2}$  are the unit vectors and  $x_1$  and  $x_2$  Cartesian coordinates. As confirmed in Ref.<sup>18</sup>, the vectors given in Eq. (80) are the fundamental translation vectors of the  $s1$  effective lattice.

#### D. The two-component quantum liquid of charge $c$ fermions and spin-neutral two-spinon $s1$ fermions

In the case of  $x \geq 0$ ,  $m = 0$ , and  $N_{s1}^h = 0$  ground states of the model on the square lattice whose  $s1$  momentum band is full and all  $N_{a_{s1}}^2$  sites of the  $s1$  effective lattice are occupied we consider that the square root  $N_{a_s}$  of the number  $N_{a_s}^2$  of sites of the spin effective lattice is an integer so that the spin effective lattice is a square lattice with  $N_{a_s} \times N_{a_s}$  sites. It follows that the square root  $N_{a_{s1}}$  of the number  $N_{a_{s1}}^2$  of sites of the  $s1$  effective lattice cannot in general be an integer number yet  $N_{a_{s1}}^2$  is. However, within the  $N_a^D \gg 1$  limit considered here and as mention above for general  $\alpha\nu$  branches, we use the notation  $N_{a_{s1}}^D$  for the number of sites of the  $s1$  effective lattice where  $D = 1$  and  $D = 2$  for the model on the 1D and square lattice, respectively.

For the one- and two-electron subspace as defined in this paper the number  $N_{a_{s1}}^D$  of sites of the  $s1$  effective lattice and  $s1$  band discrete momentum values,  $N_{s1}$  of  $s1$  fermions, and  $N_{s1}^h$  of  $s1$  fermion holes have expressions given in Eq. (76). The corresponding numbers for the  $c$  effective lattice and  $c$  band are provided in Eq. (77). For that subspace the  $s1$  band is either full by  $N_{s1} = N_{a_{s1}}^D = 2S_c = N_{a_s}^D/2$   $s1$  fermions or has one or two holes. Furthermore, one-electron and two-electron excitations have no overlap with excited states with two holes and one hole in the  $s1$  band, respectively. Hence as given in Table I excited states with a single hole in the  $s1$  band correspond to one-electron excitations and those with  $N_{s1}^h = 0, 2$  holes in that band refer to two-electron excitations. Excited states with  $N_{s1}^h = 3$  (and  $N_{s1}^h = 4$ ) holes in the  $s1$  momentum band correspond to very little one-electron (and two-electron) spectral weight and are ignored within our definition of one- and two-electron subspace.

According to the number value ranges of Eqs. (72) and (73) and number values provided in Table I, the one- and two-electron subspace is spanned by excited states having either none  $N_{s2} = 0$  or one  $N_{s2} = 1$  spin-neutral four-spinon  $s2$  fermion. When  $N_{s2} = 1$  there are no independent spinons and one finds for the  $N_{s2} = 1$  states spanning that subspace that  $N_{a_{s2}}^D = 1$  for  $N_{s2} = 1$  so that the  $s2$  fermion occupies a  $s2$  band with a single vanishing momentum value and hence  $N_{s2}^h = 0$  holes. Indeed, when  $N_{s2} = 1$  the  $s2$  fermion has vanishing energy and momentum and consistently with Eq. (41) is for  $H = 0$  invariant under the electron - rotated-electron unitary transformation. Therefore, the only effect of its creation and annihilation is on the numbers of occupied and unoccupied sites of the  $s1$  effective lattice and corresponding numbers of  $s1$  band  $s1$  fermions and  $s1$  fermion holes. Specifically, according to the expressions provided in Eq. (76) and number values of Table I the deviations  $\delta S_c = \delta S_s = 0$  and  $\delta N_{s2} = 1$  generated by a state transition involving creation of one  $s2$  fermion lead to deviations in the number of  $s1$  fermions and  $s1$  fermion holes given by  $\delta N_{s1} = -2\delta N_{s2} = -2$  and  $\delta N_{s1}^h = 2\delta N_{s2} = 2$ , respectively.

It follows that for  $N_{s2} = 1$  excited states one has from the ranges of Eqs. (72) and (73) and number values of Table I that  $S_s = 0$  so that according to Eq. (76) the number of holes of the  $s1$  band is given by  $N_{s1}^h = 2N_{s2} = 2$ , in contrast to  $N_{s1}^h = 0$  for the initial ground state. This is consistent with what was mentioned previously: Upon creation onto the ground state of a  $s2$  fermion the number  $N_{a_{s1}}^D$  of sites of the  $s1$  effective lattice remains unaltered and following the annihilation of two  $s1$  fermions and creation of one  $s2$  fermion two unoccupied sites appear in it and hence two holes emerge in the  $s1$  band. The emergence of these unoccupied sites and holes involves two virtual processes where (i) two  $s1$  fermions are annihilated and four independent spinons are created and (ii) the latter independent spinons are annihilated and the  $s2$  fermion is created.

The only net effect of creation of the vanishing-energy and zero-momentum  $s2$  fermion is the annihilation of two  $s1$  fermions and corresponding emergence of two holes in the  $s1$  band and two unoccupied sites in the  $s1$  effective lattice. Therefore, in the case of the one- and two-electron subspace one can ignore that object in the theory provided that the corresponding changes in the  $s1$  band and  $s1$  effective lattice occupancies are accounted for. For excited states with a single  $s2$  fermion two of the four spinons of such an object are used within neutral  $s1$  fermion particle-hole excitations in the motion of  $s1$  fermions around in the  $s1$  effective lattice as unoccupied sites of that lattice<sup>18</sup>, consistently with the expression  $N_{s1}^h = 2N_{s2}$  given in Eq. (76).

A similar situation occurs for the  $L_s = 2S_s$  independent spinons, whose number  $L_s = [L_{s,-1/2} + L_{s,+1/2}] = 2S_s$  belongs in the present subspace to the ranges given in Eqs. (72) and (73) and Table I such that  $2S_s = 0, 1, 2$ . For  $2S_s = 1, 2$  one has that  $N_{s2} = 0$  so that following Eq. (76) the number of unoccupied sites of the  $s1$  effective lattice and of  $s1$  fermion holes is for the excited states under consideration given by  $N_{s1}^h = 2S_s = 1, 2$ . However, in contrast

to the  $s2$  fermion, a deviation  $\delta 2S_s = 1, 2$  generated by a state transition may lead to deviations in the numbers of occupied and unoccupied sites of the  $s1$  effective lattice and corresponding  $s1$  fermion and  $s1$  fermion holes that do not obey the usual equality  $\delta N_{s1} = -\delta N_{s1}^h$ . Indeed, now  $2\delta S_c = \pm 1$  for  $\delta N_{s1}^h = 2\delta S_s = 1$  and  $2\delta S_c = 0, \pm 2$  for  $\delta N_{s1}^h = 2\delta S_s = 2$  and according to the expressions provided in Eq. (76) such deviations lead to deviations in the numbers of occupied and unoccupied sites of the  $s1$  effective lattice and corresponding numbers of  $s1$  fermions and  $s1$  fermion holes given by  $\delta N_{s1} = [\delta S_c - \delta S_s]$  and  $\delta N_{s1}^h = \delta 2S_s$ , respectively. It follows that the total number of sites and thus of discrete momentum values of the  $s1$  band may also change. That leads to an additional deviation  $\delta N_{a_{s1}}^D = [\delta S_c + \delta S_s]$ . As given in Table I, for one-electron excited states one has that  $\delta N_{s1}^h = 2\delta S_s = 1$  and  $2\delta S_c = \pm 1$  so that  $\delta N_{s1} = \pm 1/2 - 1/2 = -1, 0$  and  $\delta N_{a_{s1}}^D = \pm 1/2 + 1/2 = 0, -1$ . For  $N_{s2} = 0$  two-electron excited states one has  $\delta N_{s1}^h = 2\delta S_s = 2$  and  $2\delta S_c = 0, \pm 2$  so that  $\delta N_{s1} = -1, \pm 1 - 1 = -2, -1, 0$  and  $\delta N_{a_{s1}}^D = 1, \pm 1 + 1 = 0, 1, 2$ .

Excitations that involve changes  $\delta N_{a_{s1}}^D = [\delta S_c + \delta S_s]$  in the number of sites and discrete momentum values of the  $s1$  effective lattice and  $s1$  band, respectively, correspond for the  $s1$  fermion operators  $f_{\vec{q},s1}^\dagger$  and  $f_{\vec{q},s1}$  to transitions between different quantum problems. Indeed, such operators act onto subspaces spanned by neutral states, which conserve  $S_c$ ,  $S_s$ , and  $N_{a_{s1}}^D$ . In turn, the generator of non-neutral excitations is the product of an operator that makes small changes associated with the small variations  $\delta N_{a_{s1}}^D = [\delta S_c + \delta S_s]$  both in the  $s1$  effective lattice and corresponding  $s1$  momentum band with a  $s1$  fermion operator or a product of such operators appropriate to the excited-state subspace.

Also the vanishing momentum and energy  $L_{\eta,+1/2} = x N_a^D$  independent  $+1/2$   $\eta$ -spinons are invariant under the electron - rotated-electron unitary transformation and have no direct effect on the physics. For  $x > 0$  and the one- and two-electron subspace considered here they correspond to a single occupancy configuration associated with the  $\eta$ -spin vacuum  $|0_\eta; N_{a_\eta}^D\rangle$  of Eq. (23). In turn, the degrees of freedom of the rotated-electron occupancies of such  $x N_a^D$  sites of the original lattice associated with the  $U(1)$  symmetry refer to the  $N_c^h = x N_a^D$  unoccupied sites of the  $c$  effective lattice of Eq. (77) and corresponding  $c$  band holes. Therefore, alike for the one- and two-electron subspace the effects of creation and annihilation of a  $s2$  fermion or independent spinons are taken into account through the corresponding changes in the numbers of occupied and unoccupied sites of the  $s1$  effective lattice and corresponding  $s1$  fermion and  $s1$  fermion hole numbers, the creation and annihilation of independent  $+1/2$   $\eta$ -spinons has no effects on the physics except that their number equals that of unoccupied sites of the  $c$  effective lattice and  $c$  band holes.

In summary, when acting onto the one- and two-electron subspace as defined in Subsection V-A, the Hubbard model refers to a two-component quantum liquid described in terms of two types of objects on the corresponding effective lattices and momentum bands: The charge  $c$  fermions and spin-neutral two-spinon  $s1$  fermions. For the model on the square lattice that is the square-lattice quantum liquid further studied in Refs.<sup>1,22</sup>. The presence of independent  $+1/2$  spinons or a composite  $s2$  fermion is taken into account through the numbers of occupied and unoccupied sites of the  $s1$  effective lattice and corresponding  $s1$  fermion and  $s1$  fermion holes, whereas the number of independent  $+1/2$   $\eta$ -spinons equals that of the unoccupied sites of the  $c$  effective lattice and  $c$  band holes. Otherwise, the presence of vanishing momentum and energy independent  $+1/2$  spinons, spin-neutral four-spinon  $s2$  fermion, and independent  $+1/2$   $\eta$ -spinons has no effects on the physics. This property follows from all such objects being invariant under the electron - rotated-electron unitary transformation.

Spin-singlet excitations generated by application onto a  $m = 0$  and  $x \geq 0$  initial ground state of the operator  $f_{0,s2}^\dagger f_{\vec{q},s1} f_{\vec{q}',s1}$  where  $\vec{q}$  and  $\vec{q}'$  are the momenta of the two emerging  $s1$  fermion holes are neutral states which conserve  $S_c$ ,  $S_s$ , and  $N_{a_{s1}}^D$ . (See Table I.) For the model on the square lattice the role of the  $s2$  fermion creation operator  $f_{0,s2}^\dagger$  is exactly canceling the contributions of the annihilation of the two  $s1$  fermions of momenta  $\vec{q}$  and  $\vec{q}'$  to the commutator  $[\hat{q}_{s1\ x1}, \hat{q}_{s1\ x2}]$  of the  $s1$  translation generators in the presence of the fictitious magnetic field  $\vec{B}_{s1}$  of Eq. (25), so that the overall excitation is neutral. Since the  $s2$  fermion has vanishing energy and momentum and the  $s1$  band and its number  $N_{a_{s1}}^2$  of discrete momentum values remain unaltered, one can effectively consider that the generator of such an excitation is  $f_{\vec{q},s1} f_{\vec{q}',s1}$  and omit the  $s2$  fermion creation, whose only role is assuring that the overall excitation is neutral and the two components of the  $s1$  fermion microscopic momenta can be specified. It follows that for the one- and two-electron subspace the operators  $f_{\vec{q},s1} f_{\vec{q}',s1}$ ,  $f_{\vec{q}',s1}^\dagger f_{\vec{q},s1}^\dagger$ ,  $f_{\vec{q},s1}^\dagger f_{\vec{q}',s1}$ , and  $f_{\vec{q},s1} f_{\vec{q}',s1}^\dagger$  generate neutral excitations.

The quantum-liquid  $c$  fermions are  $\eta$ -spinless and spinless objects without internal degrees of freedom and structure whose effective lattice is identical to the original lattice. For the complete set of energy eigenstates that span the Hilbert space the occupied sites (and unoccupied sites) of the  $c$  effective lattice correspond to those singly occupied (and doubly occupied and unoccupied) by the rotated electrons. The corresponding  $c$  band has the same shape and momentum area as the first Brillouin zone.

In contrast, the quantum-liquid composite spin-neutral two-spinon  $s1$  fermions have internal structure and the definition of the  $s1$  effective lattice in terms of both the original lattice and the spin effective lattice as well as the spinon occupancy configurations that describe such objects is for the one- and two-electron subspace a more complex problem, which deserves and requires further studies<sup>18</sup>. It is simplified by the property that the  $s1$  fermion occupancy

configurations of the states that span the one- and two-electron subspace refer to a  $s1$  effective lattice with none, one, or two unoccupied sites. Also the shape of the corresponding  $s1$  momentum band and corresponding boundary and the form of the  $c$  and  $s1$  energy dispersions are complex unsolved problems investigated in Ref.<sup>1</sup>.

## VI. LONG-RANGE ANTIFERROMAGNETIC ORDER AND SHORT-RANGE SPIN ORDER OF THE MODEL ON THE SQUARE LATTICE FOR $x = 0$ AND $0 < x < x_*$ , RESPECTIVELY

Here we profit from the rotated-electron description introduced in this paper to study the occurrence at zero temperature of a long-range antiferromagnetic order and a short-range spin order in the Hubbard model on the square lattice at  $x = 0$  and for a well defined range of finite hole concentrations, respectively. For small hole concentrations  $0 < x \ll 1$  and intermediate and large  $U/4t$  values the latter order has a spiral-incommensurate character<sup>27</sup>.

### A. Extension of the Mermin and Wagner Theorem to the half-filling Hubbard model for $U/4t > 0$

We recall that for  $U/4t \gg 1$  the spin degrees of freedom of the half-filling Hubbard model on a square lattice are described by a spin-1/2 isotropic Heisenberg model on a square lattice. It follows that the Mermin and Wagner Theorem<sup>48</sup> is valid for the former model at half filling and  $U/4t \gg 1$ . The theorem states that then there is no long-range antiferromagnetic order for finite temperatures  $T > 0$ .

Let us provide evidence that the Mermin and Wagner Theorem applies to the half-filling Hubbard model on a square lattice for all values  $U/4t > 0$ . The possibility of such an extension to  $U/4t > 0$  is strongly suggested by evidence involving the transformation laws of the spin configurations under the electron - rotated-electron unitary transformation. We recall that in terms of rotated electrons, the occupancy configurations that generate the energy eigenstates are the same for all finite values  $U/4t > 0$ . Moreover, such rotated-electron occupancy configurations equal those that generate such states in terms of electrons in the  $U/4t \rightarrow \infty$  limit.

However, the electronic occupancy configurations that in the  $U/4t \rightarrow \infty$  limit generate the energy eigenstates that span the one- and two-electron subspace associated with our description correspond to an involved problem. Indeed, the suitable objects whose occupancy configurations that generate such states have a simple form, rather than the electrons, are the “quasicharges”, spins, and pseudospins of Ref.<sup>12</sup>, which are our  $c$  fermion holes, spinons, and  $\eta$ -spinons, respectively, in that limit. For the model on the square lattice in the one- and two-electron subspace the energy bandwidths of the  $\alpha\nu$  fermion dispersions vanish for  $x > 0$  in the  $U/4t \rightarrow \infty$  limit and the  $c$  fermion dispersion has for  $0 < x < 1$  the simple form  $\epsilon_c(\vec{q}) = -2t \sum_{i=1}^2 [\cos(q_{x_i}) - \cos(q_{Fcx_i})]$  in terms of the  $c$  band momentum components<sup>1</sup>.

The use of the following two properties provides below strong evidence that the Mermin and Wagner Theorem holds for the half-filling Hubbard model on the square lattice for  $U/4t > 0$ : I) The  $x = 0$  and  $m = 0$  absolute ground state is invariant under the electron - rotated-electron unitary transformation<sup>1</sup> so that the occurrence of long-range antiferromagnetic order for  $U/4t \rightarrow \infty$ , associated with that of the spin-1/2 isotropic Heisenberg model, implies the occurrence of that long-range order for  $U/4t > 0$  as well; II) Since in terms of rotated electrons for  $U/4t > 0$  single and double occupancy are good quantum numbers, the rotated-electron occupancy configurations that generate the energy eigenstates are more ordered than the corresponding electron occupancy configurations. It follows that the lack of long-range antiferromagnetic order in terms of the spins of the rotated electrons implies as well a lack of such an order in terms of the spins of the electrons whose occupancy configurations generate the same states.

We recall that the rotated-electron occupancy configurations that for  $U/4t > 0$  generate the energy eigenstates are identical to the electron occupancy configurations that for  $U/4t \rightarrow \infty$  generate the energy eigenstates belonging to the same  $V$  tower. Hence concerning the original-lattice rotated-electron occupancies, the Mermin and Wagner Theorem applies to all finite values of  $U/4t > 0$ : for the occupancy configurations of the rotated-electron spins there is no long-range antiferromagnetic order for temperatures  $T > 0$ . That the lack of long-range antiferromagnetic order for  $U/4t > 0$  and  $T > 0$  of the rotated-electron spins implies a similar lack of such an order for the spins of the original electrons follows from the above property II, being consistent with for finite values of  $U/4t$  the spin occupancy configurations being more ordered for the rotated electrons than for the electrons.

This is also consistent with the existence of long-range antiferromagnetic order for the Hubbard model on a square lattice at hole concentration  $x = 0$ , temperature  $T = 0$ , and  $U/4t > 0$  only, associated with that of the  $x = 0$  and  $m = 0$  absolute ground state, which the above property I refers to, in agreement with the numerical results of Refs.<sup>49,50</sup>. As discussed below, there is strong evidence that for  $x = 0$ ,  $T > 0$ , and  $U/4t > 0$  such an order is replaced by a short-range spin order.

Since the electron - rotated-electron unitary operator  $\hat{V}$  does not commute with the Hamiltonian, the rotated-electron occupancy configurations that generate the energy eigenstates are for  $U/4t > 0$  the same as for  $U/4t \rightarrow \infty$



in terms of electrons. However the corresponding energies depend on the value of  $U/4t$ . It turns out that the rotated-electron occupancy configurations associated with the long-range antiferromagnetic order refer to a subspace that for  $U/4t$  finite exists below an energy given by the energy scale  $\mu^0$ , Eq. (34). Such a subspace is spanned by energy eigenstates with  $N_{a_\eta}^2 = [N_a^2 - 2S_c] = 0$  and  $N_{a_s}^2 = 2S_c = N_a^2$  sites so that there is no  $\eta$ -spin effective lattice and the spin effective lattice has as many sites as the original lattice and is identical to it. In such a subspace there are no rotated-electron doubly occupied sites and no rotated-electron unoccupied sites.

The point is that the number of sites of the spin effective lattice being given by  $N_{a_s}^2 = N_a^2$  is a necessary condition for the occurrence of long-range antiferromagnetic order: Concerning the spins of the rotated-electron occupancy configurations such an order occurs when the  $\eta$ -spin effective lattice does not exist and the quantum-system vacuum (23) becomes  $|0_s\rangle = |0_s; N_a^D\rangle \times |GS_c; N_a^D\rangle$  and the system global symmetry is  $U(2)/Z_2 = SO(3) \times U(1)$ . For  $U/4t \rightarrow \infty$  when the spin degrees of freedom of the half-filling Hubbard model are described by the Heisenberg model, the subspace for which  $N_{a_s}^2 = N_a^2$  describes the whole finite-energy physics. This follows from according to Eq. (34) the energy scale  $\mu^0$  being given by  $\mu^0 = U/2 \rightarrow \infty$ . However, for finite  $U/4t > 0$  one has that the spin occupancy configurations in a spin effective lattice with  $N_{a_s}^2 = N_a^2$  sites, which are expected to be behind the long-range antiferromagnetic order, exist only for energies below  $\mu^0$ . The Mott-Hubbard gap  $2\mu^0$ , which refers to the charge degrees of freedom, affects the spin degrees of freedom as well:  $\mu^0$  is the energy above which the  $\eta$ -spin effective lattice emerges and hence the number of sites of the spin effective lattice decreases so that  $N_{a_s}^2 < N_a^2$ . It follows that for the Hubbard model on a square lattice  $\mu^0$  is the energy below which the long-range antiferromagnetic order of the rotated-electron spins survives for  $x = 0$ ,  $m = 0$ , and temperature  $T = 0$ .

Finally, it follows from the above property II that since the ground-state rotated-electron occupancy configurations are for finite values of  $U/4t$  more ordered than those of the electrons for the same state, a lack of long-range antiferromagnetic order of the rotated-electron spins for  $N_{a_s}^2 < N_a^2$  implies a similar lack of long-range antiferromagnetic order for the spins of the original electrons. In contrast to the  $x = 0$  and  $m = 0$  absolute ground state of property I,  $0 < x < 1$  and  $m = 0$  ground states are not invariant under the electron - rotated-electron unitary transformation.

### B. Short-range spin order of the model on the square lattice for $m = 0$ and $0 < x \ll 1$

The requirement for the occurrence of long-range antiferromagnetic order at zero temperature  $T = 0$  in the Hubbard model on the square lattice that the number of sites of the  $\eta$ -spin and spin effective lattices are given by  $N_{a_\eta}^2 = 0$  and  $N_{a_s}^2 = N_a^2$ , respectively, implies that there is no such a long-range order for  $m = 0$ ,  $x > 0$ , and  $T = 0$ . Indeed, then  $2S_c < N_a^2$  so that  $N_{a_\eta}^2 = [N_a^2 - 2S_c] > 0$  and  $N_{a_s}^2 = 2S_c < N_a^2$ . For the one- and two-electron subspace such expressions read  $N_{a_\eta}^2 = x N_a^2 > 0$  and  $N_{a_s}^2 = (1 - x) N_a^2 < N_a^2$ , respectively.

One may use as zero-temperature order parameter of the  $m = 0$  and  $x = 0$  quantum phase the excitation energy  $\mu^0$  below which the long-range antiferromagnetic order survives, whose limiting behaviors for  $U/4t \ll 1$  and  $U/4t \gg 1$  are given in Eq. (34) for  $D = 2$ . In addition to those, here we provide an approximate formula valid for intermediate  $U/4t$  values  $u_0 \leq U/4t \leq u_1$ ,

$$\begin{aligned} \mu^0 &\approx 32 t e^{-\pi \sqrt{\frac{4t}{U}}} , \quad U/4t \ll 1 , \\ &\approx \frac{2e^1 t}{\pi} \sqrt{1 + (U/4t - u_0)} , \quad u_0 \leq U/4t \leq u_1 , \\ &\approx [U/2 - 4t] ; \quad U/4t \gg 1 , \end{aligned} \tag{81}$$

where the behavior  $\mu_0(U/4t) \approx \mu_0(u_0) \sqrt{1 + (U/4t - u_0)}$  is expected to be a good approximation for the small range  $u_0 \leq U/4t \leq u_1$ ,  $u_0 \approx 1.302$ , and  $u_1 \approx 1.600$ . The approximate magnitude  $\mu_0(u_0) \approx [2e^1/\pi] t$  is that consistent with the relation  $\mu_0(u_0) \approx \mu_0(u_*)/\sqrt{1 + (u_* - u_0)}$  where  $u_0 = 1.302$  is the  $U/4t$  value at which the energy parameter  $\Delta_0$  is found below to reach its maximum magnitude and  $u_* = 1.525$  is that for which the studies of Ref.<sup>1</sup> lead by a completely different method to  $\mu_0(u_*) \approx 566 \text{ meV}$  for  $t = 295 \text{ meV}$  and  $U/4t \approx u_* = 1.525$ . The use of  $\mu_0(u_0) \approx [2e^1/\pi] t$  in the formula  $\mu_0(U/4t) \approx \mu_0(u_0) \sqrt{1 + (U/4t - u_0)}$  leads for  $t = 295 \text{ meV}$ ,  $U/4t \approx u_* = 1.525$ , and  $u_0 = 1.302$  to nearly the same magnitude,  $\mu_0(u_*) \approx 565 \text{ meV}$ .

There is strong evidence of the occurrence in the half-filling Hubbard model on the square lattice of strong short-range antiferromagnetic correlations for  $T > 0$  and below a crossover temperature called  $T_x$  in Ref.<sup>29</sup>, which here we denote by  $T_0^*$ . This is consistent with then the system being driven into a phase with short-range spin order. Furthermore, that the occurrence of long-range antiferromagnetic order requires  $T = 0$ ,  $N_{a_\eta}^2 = 0$ , and  $N_{a_s}^2 = N_a^2$  is consistent with the short-range spin order occurring for  $m = 0$ ,  $0 < x \ll 1$ , and  $0 \leq T < T_0^*$  being similar to that occurring for  $m = 0$ ,  $x = 0$ , and  $0 < T < T_0^*$  and was studied previously in Ref.<sup>29</sup> for  $0 < T \ll T_0^*$ .

One may choose the excitation energy  $2\Delta_0$  below which the short-range spin order with strong antiferromagnetic correlations survives to play the role of zero-temperature order parameter of the quantum phase displaying such an order occurring for  $m = 0$  and  $0 < x \ll 1$ . That energy parameter has a  $U/4t$  dependence qualitatively similar to that of the energy scale  $2k_B T_0^*$ , with the equality  $2\Delta_0 \approx 2k_B T_0^*$  holding approximately. For both vanishing and finite temperatures a phase displaying a short-range spiral-incommensurate spin order occurs for (i)  $m = 0$ ,  $0 < x \ll 1$ , and  $0 \leq T \ll T_0^*$  and (ii)  $m = 0$ ,  $x = 0$ , and  $0 < T \ll T_0^*$ . At  $m = 0$  and temperatures below  $T_0^*$  the system is driven both for (i)  $0 < x \ll 1$  and  $0 \leq T < T_0^*$  and (ii)  $x = 0$  and  $0 < T < T_0^*$  into a renormalized classical regime where the  $x = 0$  and  $T = 0$  long-range antiferromagnetic order is replaced by such a short-range spin order, which is a quasi-long-range spin order as that studied in Ref.<sup>51</sup> for simpler spin systems.

Let us study the  $U/4t$  dependence of  $\Delta_0 \approx k_B T_0^*$  by combining the results obtained from the use of the general description introduced in this paper with those of the low-temperature approach to the half-filled model of Ref.<sup>29</sup>, whose investigations focus on temperatures  $0 < T \ll T_0^*$ . We use often in the following the magnitudes of the energy bandwidth  $W_{s1}^0$  and energy parameter  $\mu_0$  derived in Ref.<sup>1</sup> For the value  $U/4t \approx 1.525$  found in Ref.<sup>32</sup> to be appropriate to the description of the properties of several hole-doped cuprates on combining the description introduced in this paper with results on the spin-wave dispersion of the half-filled Hubbard model in a spin-density-wave-broken symmetry ground state obtained by summing up an infinite set of ladder diagrams<sup>30</sup>.

The picture that emerges is that for the Hubbard model on a square lattice at  $T = 0$  there is an overall zero-temperature energy order parameter  $2|\Delta|$ , which at  $x = 0$  has a singular behavior due to a sharp quantum phase transition occurring at vanishing hole concentration, such that there is long-range antiferromagnetic order at  $x = 0$  and, as justified below by combining our description with the results of Refs.<sup>1,23,27</sup>, a short-range spiral-incommensurate spin order for  $0 < x \ll 1$ . Consistently, the energy scale  $2|\Delta|$  reads,

$$2|\Delta| = \mu^0, \quad x = 0; \quad 2|\Delta| \approx 2\Delta_0 \left(1 - \frac{x}{x_*^0}\right), \quad 0 < x \ll 1, \quad U/4t \geq u_0 \approx 1.302. \quad (82)$$

The linear dependence of  $2|\Delta| \approx 2\Delta_0(1 - x/x_*^0)$  on  $x$  where  $x_*^0 \approx 2r_s/\pi$  and  $r_s = \Delta_0/4W_{s1}^0$  is justified in Ref.<sup>1</sup>. Hence  $2|\Delta|_{x=0} = \mu^0$  is for  $U/4t > 0$  different from  $2\Delta_0 = \lim_{x \rightarrow 0} 2|\Delta|$ . Symmetry arguments imply that  $\lim_{U/4t \rightarrow 0} 2\Delta_0 = 2|\Delta|_{x=0} = \mu^0$  so that the two energy scales become the same in that limit.

The energy scale  $\Delta_0$  is found in Refs.<sup>1,22</sup> to play an important role in the square-lattice quantum-liquid physics. Upon increasing  $U/4t$ , it interpolates between  $\Delta_0 \approx \mu^0/2 \approx 16t e^{-\pi\sqrt{4t/U}}$  for  $U/4t \ll 1$  and  $\Delta_0 \approx 4W_{s1}^0 \approx \pi[4t]^2/U$  for  $U/4t \gg 19$ , going through a maximum magnitude at a  $U/4t$  value found below to be approximately given by  $U/4t = u_0 \approx 1.302$ . The energy parameter  $\mu_0/2$  is an increasing function of  $U/4t$ . As given in Eq. (81), it behaves as  $\mu_0/2 \approx 16t e^{-\pi\sqrt{4t/U}}$  for  $U/4t \ll 1$  and as  $\mu_0/2 \approx [U/2 - 4t]$  for  $U/4t \gg 1$ . In turn, the energy scale  $4W_{s1}^0$  is a decreasing function  $U/4t$ , which according to Eq. (38) is for  $D = 2$  given by  $4W_{s1}^0 = 16t$  at  $U/4t = 0$  and decreases approximately as  $4W_{s1}^0 \approx \pi[4t]^2/U$  for very large  $U/4t$ . The energy scale  $\Delta_0$  interpolates between these two behaviors, vanishing both for  $U/4t \rightarrow 0$  and  $U/4t \rightarrow \infty$  as  $\Delta_0 \approx 16t e^{-\pi\sqrt{4t/U}}$  and  $\Delta_0 \approx \pi(4t)^2/U$  where it becomes  $\mu_0/2$  and an energy scale  $\pi(4t)^2/U$  associated with the strong  $0 < x \ll 1$  antiferromagnetic correlations, respectively. This is consistent with its maximum magnitude being reached at the intermediate  $U/4t$  value  $U/4t = u_0$  for which  $\mu_0/2 \approx 4W_{s1}^0$  and we consider that such a  $U/4t$  value is that at which the equality  $\mu_0(u_0)/2 = 4W_{s1}^0(u_0)$  holds.

The ratio  $r_s = \Delta_0/4W_{s1}^0$  is parametrized in the following as  $r_s = e^{-\lambda_s}$  where  $\lambda_s = |\ln(\Delta_0/4W_{s1}^0)|$  has an important role in such an interpolation behavior. The energy scale  $\Delta_0$  can then be expressed as,

$$\Delta_0 = r_s 4W_{s1}^0 = 4W_{s1}^0 e^{-\lambda_s}; \quad \lambda_s = |\ln(\Delta_0/4W_{s1}^0)|, \quad (83)$$

where  $\lambda_s$  has the limiting behaviors,

$$\lambda_s = \pi\sqrt{4t/U}, \quad U/4t \ll 1; \quad \lambda_s \approx 4t u_0/U, \quad u_{00} \leq U/4t \leq u_1; \quad \lambda_s = 0, \quad U/4t \rightarrow \infty, \\ u_{00} \approx (u_0/\pi)^2 \approx 0.171; \quad u_0 \approx 1.302; \quad u_1 \approx 1.600. \quad (84)$$

Consistently, the ratio  $r_s$  is an increasing function of  $U/4t$ , which changes continuously from  $r_s = 0$  for  $U/4t \rightarrow 0$  to  $r_s = 1$  for  $U/4t \rightarrow \infty$ . That for  $u_{00} \leq U/4t \leq u_1$  it is approximately given by  $r_s \approx e^{-4t u_0/U}$  instead of  $r_s \approx e^{-\pi\sqrt{4t/U}}$  for  $U/4t \ll 1$  is consistent with for large  $U/4t$  it being such that  $(1 - r_s) \propto 4t/U$  rather than  $(1 - r_s) \propto \sqrt{4t/U}$ .

The temperature  $T_x$  which plays the role of  $T_0^* \approx \Delta_0/k_B$  is plotted in Fig. 3 of Ref.<sup>29</sup>. Its  $U/4t$  dependence is qualitatively correct,  $T_x$  vanishing both in the limits  $U/4t \rightarrow 0$  and  $U/4t \rightarrow \infty$  and going through a maximum magnitude at an intermediate value  $5/4 < U/4t < 3/2$ . Nevertheless, the interpolation function used to produce it, provided in Ref. 74 of such a paper, is poor for intermediate values of  $U/4t$ . However, that does not affect the validity of the results of Ref.<sup>29</sup>. Indeed, the studies of that reference refer to the temperature range  $0 < T \ll T_x$  for which

the accurate dependence of  $T_x$  on  $U/4t$  is not needed and the goal of its Fig. 3 is just illustrating qualitatively the  $T_x$  behavior over the entire coupling range<sup>52</sup>.

Our goal is reaching a more quantitatively accurate  $U/4t$  dependence of the energy parameter  $\Delta_0 \approx k_B T_0^*$  for intermediate  $U/4t$  values, consistent with the qualitative physical picture of Ref.<sup>29</sup>. That according to Eqs. (83) and (84) one has that  $\Delta_0 = 4W_{s1}^0 e^{-\lambda_s}$  for  $U/4t > 0$  where the parameter  $\lambda_s$  is a continuous decreasing function of  $U/4t$  given by  $\lambda_s = \infty$  for  $U/4t \rightarrow 0$  and  $\lambda_s = 0$  for  $U/4t \rightarrow \infty$  reveals that the magnitude  $\lambda_s = 1$  separates two physical regimes. Consistently,  $\lambda_s = 1$  refers to the  $U/4t$  value  $U/4t = u_0$  at which  $\Delta_0$  reaches its maximum magnitude  $\max\{\Delta_0\} = [\mu_0(u_0)/2] e^{-1} = 4W_{s1}^0(u_0) e^{-1}$ .

That as found in Ref.<sup>1</sup>, both the parameter  $x_*^0$  is for approximately  $u_0 \leq U/4t \leq u_1$  given by  $x_*^0 = 2r_s/\pi = 2e^{-4t u_0/U}/\pi$  and at  $U/4t \approx u_* = 1.525$  reads  $x_*^0 \approx 0.27$  implies that  $u_0 \approx 1.3$ . Moreover, in that reference it is found that  $4W_{s1}^0(u_*) = [198.4/295]t \approx 0.673t$  at  $U/4t \approx u_* = 1.525$ . Since  $W_{s1}^0 = \lim_{x \rightarrow 0} W_{s1}$  has the same magnitude as the  $x = 0$  energy bandwidth  $W_{s1}$ , such a result is obtained in that reference from comparison of the  $x = 0$  and  $m = 0$  spin excitation spectra for the high symmetry directions found by use of the description introduced in this paper with those estimated by the controlled approximation of Ref.<sup>30</sup>. On combining the equality  $\mu_0(u_0)/2 = 4W_{s1}^0(u_0)$  with the magnitude  $\mu_0(u_0) \approx [2e^1/\pi]t$  of Eq. (81) we find  $4W_{s1}^0(u_0) \approx [e^1/\pi]t \approx 1.731t$  and  $\max\{\Delta_0\} = [\mu_0(u_0)/2] e^{-1} = 4W_{s1}^0(u_0) e^{-1} \approx t/\pi$ .

Note that the magnitude  $W_{s1}^0(u_*) = [49.6/295]t \approx 0.168t$  obtained in Ref.<sup>1</sup> is about 12.25 times smaller than that found by use of the limiting expression  $4\pi t^2/U \approx 2.060t$  at  $U/4t = 1.525$ . This reveals that for the Hubbard model on the square lattice such a limiting expression is valid for a smaller range of very large  $U/4t$  values than for 1D. Specifically, we find that it is valid for  $U/4t \gg 19$ . The value  $U/4t \approx 18.70 \approx 19$  is that at which  $4\pi t^2/U$  is given by  $0.168t$ , alike  $W_{s1}^0$  at  $U/4t \approx 1.525$ . Therefore, the relation  $W_{s1}^0 = J \approx 4\pi t^2/U$  is indeed valid for  $U/4t \gg 19$  and for the model on the square lattice the energy scale  $J \approx 4\pi t^2/U$  controls the physics for a smaller  $U/4t$  range than in 1D, which corresponds to very large  $U/4t \gg 19$  values. Hence the intermediate- $U/4t$  range plays a major role in the physics of that model, as confirmed by the related studies of Refs.<sup>1,22,32</sup>.

For the model on the square lattice and approximately the intermediate range  $u_0 \leq U/4t \leq u_1$  the  $U/4t$  dependence of the energy parameter  $4W_{s1}^0$  is of the form  $4W_{s1}^0 \approx [e^1/\pi]t W(U/4t)$  where  $W(u)$  is an unknown function of  $u = U/4t$  such that  $W(u_0) = 1$ . Since on combining Eqs. (83) and (84) one finds  $\Delta_0 = 4W_{s1}^0 e^{-4t u_0/U}$ , fulfillment of the maximum condition  $\partial\Delta_0(u)/\partial u = 0$  at  $u = u/4t = u_0$  requires the function  $W(u)$  be given by  $W(u) \approx (2 - u/u_0)$  for  $0 \leq [(u - u_0)/(u_1 - u_0)] \ll 1$ . In turn, the use of the above results  $4W_{s1}^0(u_*) = [198.4/295]t \approx 0.673t$  and  $4W_{s1}^0(u_0) \approx [e^1/\pi]t \approx 1.731t$  reveals that the ratio  $4W_{s1}^0(u_*)/4W_{s1}^0(u_0)$  may be expressed as  $4W_{s1}^0(u_*)/4W_{s1}^0(u_0) \approx [1 - (u_* - u_0)]$  so that  $W(u) \approx [1 - (u - u_0)]$  for  $u \approx u_* = 1.525$ . We then use a suitable interpolation function for  $W(u)$ , which has these two limiting behaviors, so that the energy parameter  $4W_{s1}^0$  is for  $U/4t$  intermediate values  $U/4t \in (u_0, u_1)$  given approximately by,

$$\begin{aligned} 4W_{s1}^0 &\approx \frac{e^1 t}{\pi} W(U/4t); \quad W(u) \approx 1 - (u - u_0) e^{-\frac{u_* - u}{u_* - u_0} \ln(u_0)}, \quad u_0 \leq U/4t \leq u_1, \\ u_0 &\approx u_* - 1 + e^{-1} \pi \frac{198.4}{295} \approx 1.302; \quad u_* \approx 1.525. \end{aligned} \quad (85)$$

The value  $u_0 \approx 1.302$  is that obtained from the equation  $4W_{s1}^0(u_*) = [e^1 t/\pi] [1 - (u_* - u_0)] = [198.4/295]t \approx 0.673t$ .

On combining the above results we find the following magnitudes for the energy parameter  $\Delta_0$ ,

$$\begin{aligned} \Delta_0 &\approx 16t e^{-\pi \sqrt{4t/U}}, \quad U/4t \ll 1, \\ &= \max\{\Delta_0\} \approx t/\pi, \quad U/4t = u_0, \\ &\approx e^{(1-4t u_0/U)} [t/\pi] W(U/4t), \quad u_0 \leq U/4t \leq u_1, \\ &= 4W_{s1}^0 \approx \pi [4t]^2/U, \quad U/4t \gg 19, \end{aligned} \quad (86)$$

where  $W(U/4t)$  is the interpolation function given in Eq. (85). Note that  $\partial\Delta_0(u)/\partial u = 0$  at  $u = u/4t = u_0$ , consistently with  $\Delta_0$  reaching its maximum magnitude  $t/\pi$  at that  $U/4t$  value. The overall  $U/t$  dependence of  $T_0^* \approx \Delta_0/k_B$  is similar to that plotted in Fig. 3 of Ref.<sup>29</sup> for  $T_x$  with the  $U/t$  value at which the maximum magnitude is reached shifted from  $U/t \approx 5.60$  to  $U/t \approx 5.21$  and that magnitude lessened from  $\max\{k_B T_x\} \approx 0.625t$  to  $\max\{k_B T_0^*\} \approx \max\{\Delta_0\} \approx t/\pi \approx 0.318t$ . Otherwise, such a dependence has qualitatively a shape similar to that illustrated in the figure.

Next let us provide strong evidence that for intermediate and large values of  $U/4t$  and small hole concentrations  $0 < x \ll 1$  the short-range spin order of the  $m = 0$  ground state corresponds to that of a spin-singlet incommensurate spiral state. In terms of the rotated-electron spins occupancy configurations the ground state is then a spin-singlet incommensurate spiral state for  $U/4t > 0$ ,  $m = 0$ , and  $0 < x \ll 1$ . That evidence is found on combining the above result that such a ground state is a spin-singlet state with the recent results of Ref.<sup>27</sup> concerning the spin degrees of freedom of a related quantum problem.

As discussed in Section II, for intermediate and large values of  $U/4t$  the Hubbard model on the square lattice given in Eqs. (1) and (4) in terms of electron and rotated-electron operators, respectively, can for  $D = 2$  be mapped onto an effective  $t - J$  model on a square lattice with  $t$ ,  $t' = t'(U/4t)$ , and  $t'' = t''(U/4t)$  transfer integrals where the role of the processes associated with  $t' = t'(U/4t)$  and  $t'' = t''(U/4t)$  becomes increasingly important upon decreasing the  $U/4t$  value. Rigorous results on the spin degrees of freedom of the  $t - J$  model on a square lattice with  $t$ ,  $t'$ , and  $t''$  transfer integrals were recently achieved in Ref.<sup>27</sup>. The investigations of that paper refer to small values of the hole concentration  $0 < x \ll 1$  and spin density  $m = 0$  and have as starting point a suitable action first introduced in Ref.<sup>26</sup>. The use in Ref.<sup>27</sup> of a staggered  $CP^1$  representation for the spin degrees of freedom allows to resolve exactly the constraint against double occupancy, which is equivalent to performing the electron - rotated-electron unitary transformation. In order to achieve the rigorous result that for small hole concentrations there occurs an incommensurate-spiral spin order, the effective action for the spin degrees of freedom is reached after integrating out the charge fermionic degrees of freedom and the magnetic fast  $CP^1$  modes. Importantly, the dependence on the hole-concentration of the coupling constants of the effective field theory is obtained explicitly for small  $x$ .

From the mapping between the above effective  $t - J$  model and the Hubbard model of Eqs. (1) and (4) in the subspace with vanishing rotated-electron double-occupancy, the studies of Ref.<sup>27</sup> reveal that for intermediate and large values of  $U/4t$ , spin-density  $m = 0$ , and small hole concentrations  $0 < x \ll 1$  the ground state is an incommensurate spiral state. This is a rigorous result, yet the studies of Ref.<sup>27</sup> are not conclusive on whether for  $0 < x \ll 1$  the  $m = 0$  incommensurate spiral ground state has short-range or long-range spin order. However, symmetry requires that the occurrence of long-range and short-range incommensurate-spiral spin order is associated with a spin-singlet ground state and a broken-symmetry ground state without well defined spin, respectively. Therefore, combination of our above result that the  $m = 0$  and  $0 < x \ll 1$  ground state of the Hubbard model (1) is a spin-singlet state with the result of Ref.<sup>27</sup> that such a state has a short-range incommensurate-spiral spin order is consistent with for intermediate and large values of  $U/4t$  the ground state of the model being a spin-singlet state with short-range incommensurate-spiral spin order and thus strong antiferromagnetic correlations.

Moreover, in terms of rotated electrons the short-range incommensurate-spiral spin order prevails for  $U/4t > 0$ ,  $m = 0$ , and  $0 < x \ll 1$  and implies that in terms of electrons the system has a short-range spin order. Indeed and as discussed above, the ground-state rotated-electron occupancy configurations are for finite values of  $U/4t$  more ordered than those of the electrons for the same state so that a lack of long-range spin order of the rotated-electron spins for  $m = 0$  and  $0 < x \ll 1$  implies a similar lack of long-range spin order for the spins of the original electrons. The occurrence of a short-range incommensurate-spiral spin order for  $0 < x \ll 1$  is fully consistent with the occurrence for  $U/4t > 0$  of a long-range antiferromagnetic order and a short-range spin order for  $x = 0$  and  $0 < x \ll 1$ , respectively. Above the occurrence of such long-range and short-range spin orders is associated with the number of sites of the spin effective lattice obeying the relations  $N_{a_s}^2 = N_a^2$  and  $N_{a_s}^2 < N_a^2$ , respectively. In turn, here the occurrence for  $0 < x \ll 1$  of a short-range spiral-incommensurate spin order is reached by use of completely different arguments.

The energy order parameter  $2|\Delta|$  of Eq. (82) is both for  $x = 0$  and  $x > 0$  identified in the studies of Refs.<sup>1,22</sup> with the maximum pairing energy of the  $-1/2$  and  $+1/2$  spinons of a composite spin-neutral two-spinon  $s1$  fermion. Its magnitude has a singular behavior at  $x = 0$  due to the sharp quantum phase transition from a ground state with long-range antiferromagnetic order at  $x = 0$  to a state with short-range spiral-incommensurate spin order and strong antiferromagnetic correlations for  $0 < x \ll 1$ . The results of Refs.<sup>1,22</sup> extend the  $m = 0$  and  $T = 0$  short-range spin order to a well-defined range of hole concentrations  $0 < x < x_*$ . According to these results, for  $U/4t \geq u_0$  the  $x$  dependence  $2|\Delta| \approx 2\Delta_0(1 - x/x_*)^0$  given in Eq. (82) for  $0 < x \ll 1$  is valid for  $x \in (0, x_*)$  whereas for  $x > x_*$  the energy scale  $2|\Delta|$  vanishes. Here for approximately  $U/4t \in (u_0, u_\pi)$  where  $u_\pi > u_1$  is the  $U/4t$  value at which  $r_s = 1/2$  the critical hole concentration  $x_*$  equals the  $U/4t$ -dependent parameter  $x_*^0$ . For  $U/4t \geq u_0$  the studies of the above references identify it with a critical hole concentration above which there is no short-range spin order so that  $2|\Delta| \rightarrow 0$  as  $x \rightarrow x_*$ . Indeed, the energy order parameter  $2|\Delta|$  vanishes in the absence of that order. Consistently, the spinon pairing energy vanishes for the Hubbard model on the 1D lattice for which  $2|\Delta| = 0$  for the whole range of hole concentrations. The short-range incommensurate-spiral spin order discussed here for  $0 < x \ll 1$  corresponds then to a limiting case of the general short-range spin order that according to the investigations of Refs.<sup>1,22</sup> occurs for  $0 < x < x_*$ .

The form of the  $s1$  effective lattice spacing (79) is for the square-lattice model directly related to the above spin orders. Indeed, that at  $x = 0$  and  $m = 0$  the square  $s1$  effective lattice has no unoccupied sites and its spacing is given by  $a_{s1} = \sqrt{2}a$  reveals that then its periodicity has increased relative to that of both the original lattice and  $c$  effective lattice. This is because at  $x = 0$  the  $s1$  effective lattice refers to a  $\sqrt{2} \times \sqrt{2}$  reconstruction in which the periodicity of the spin-sub-system real-space structure is increased. Such an effect is consistent with the occurrence of the long-range antiferromagnetic order at  $x = 0$  and  $m = 0$ . In turn, that for  $x > 0$  and  $m = 0$  the square  $s1$  effective lattice remains having no unoccupied sites but its spacing reads instead  $a_{s1} = \sqrt{2/(1-x)}a$  is consistent with the emergence of the short-range incommensurate-spiral spin order discussed here. Furthermore, that then the  $s1$  effective-lattice spacing is given by  $a_{s1} = \sqrt{2/(1-x)}a$  implies that the  $s1$  fermion occupancy-configuration states

break the translational symmetry.

The studies of Refs.<sup>1,22</sup> reveal that for the square-lattice quantum liquid the  $s1$  bond particles associated with the  $s1$  fermions are closely related to the spin-singlet bonds of Ref.<sup>23</sup>. The investigations of Ref.<sup>22</sup> combine the description introduced in this paper with some of the results of Ref.<sup>23</sup> on a related problem to investigate the square-lattice quantum-liquid fluctuations and competing orders in the presence of a small 3D anisotropy perturbation associated with weak plane coupling. They confirm the validity of the long-range and short-range spin orders found here at  $x = 0$  and  $x > 0$ , respectively, by studying the fluctuations of the phases that control such orders.

At  $x = 0$  and  $m = 0$  the spin effective lattice is identical to the original lattice so that the two-spinon  $s1$  bonds of the  $s1$  fermions refer to the same lattice as in Ref.<sup>23</sup> and the  $s1$  effective lattice is one of its two sub-lattices. Also for  $0 < x \ll 1$  the spin effective lattice is very similar to the original lattice and the  $s1$  effective lattice spacing  $a_{s1} \approx [\sqrt{2}/(1+x/2)]a \approx \sqrt{2}a$  is close to that of the original sub-lattices. As further discussed in Ref.<sup>22</sup>, at zero temperature,  $x = 0$ , and  $m = 0$  there are in the square-lattice quantum liquid strong phase fluctuations whose action has a local compact gauge symmetry. That corresponds to the long-range antiferromagnetic phase studied above for which monopole-antimonopole pairs of the type considered in Ref.<sup>23</sup> are unbound and proliferate. For small values  $0 < x \ll 1$  the motion of the  $c$  fermions and the associated kinetic energy play the role of symmetry-breaking Higgs terms. The presence of such terms suppresses free monopoles and is behind the replacement of the long-range antiferromagnetic order at  $x = 0$  by the short-range incommensurate-spiral spin order for  $0 < x \ll 1$ .

## VII. CONCLUDING REMARKS

In this paper we have profited from the interplay of the global  $SO(3) \times SO(3) \times U(1)$  symmetry found in Ref.<sup>2</sup> for the Hubbard model on any bipartite lattice with the transformation laws of a well-defined set of operators and quantum objects whose occupancy configurations generate a complete set of  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates under a suitably chosen electron - rotated-electron unitary transformation to introduce a general description for the model on a square lattice with  $N_a^2 \gg 1$  sites. Often the problem is also addressed for the model on the 1D lattice.

Within the description introduced in this paper the above complete set of states is generated by occupancy configurations of  $c$  fermions associated with the state representations of the  $U(1)$  symmetry,  $\eta$ -spin-neutral  $2\nu$ - $\eta$ -spinon composite  $\eta\nu$  bond particles and independent  $\eta$ -spinons associated with the state representations of the  $\eta$ -spin  $SU(2)$  symmetry, and spin-neutral  $2\nu$ -spinon composite  $s\nu$  bond particles and independent spinons associated with the state representations of the spin  $SU(2)$  symmetry. The index  $\nu = 1, 2, \dots$  refers to the number of  $\eta$ -spinon or spinon pairs in each composite object. Evidence is provided in this paper that in addition to being  $S_\eta$ ,  $S_\eta^z$ ,  $S_s$ ,  $S_s^z$ ,  $S_c$ , and momentum eigenstates, for the Hubbard model on the square lattice in the one- and two-electron subspace defined in this paper such states are energy eigenstates. (For the 1D model they are energy eigenstates for the whole Hilbert space<sup>1</sup>.)

The relation of the composite  $\eta\nu$  bond particles (and  $s\nu$  bond particles) to the  $\eta$ -spinons (and spinons) has similarities with that of the composite physical particles to the quarks in chromodynamics<sup>41</sup>. Within the latter theory the quarks have color but all quark-composite physical particles are color-neutral. Here the  $\eta$ -spinon (and spinons) that are not invariant under the electron - rotated-electron unitary transformation have  $\eta$ -spin 1/2 (and spin 1/2) but the  $2\nu$ - $\eta$ -spinon (and  $2\nu$ -spinon) composite  $\eta\nu$  bond particles (and  $s\nu$  bond particles) are  $\eta$ -spin-neutral (and spin-neutral) objects. The components of the microscopic momentum values of the  $\alpha\nu$  fermions are eigenvalues of  $\alpha\nu$  translation generators  $\hat{q}_{\alpha\nu}$  of Eq. (27) in the presence of the fictitious magnetic fields  $\vec{B}_{\alpha\nu}(\vec{r}_j)$  of Eq. (25). Those are associated with extended Jordan-Wigner transformations from which the  $\alpha\nu$  fermions emerge from the corresponding  $\alpha\nu$  bond particles. In the  $U/4t \rightarrow \infty$  limit the  $\alpha\nu$  band momentum occupancy configurations that generate the energy eigenstates of Hubbard model on a square lattice in subspaces (A) and (B) defined in this paper are described by the 2D QHE physics. The structure of the spin configurations associated with a  $s1$  fermion simplifies in the one- and two-electron subspace introduced in this paper where only the charge  $c$  fermions and spin-neutral two-spinon  $s1$  fermions play an active role. The physical picture that emerges is that of a two-component quantum liquid of charge  $c$  fermions and spin-neutral two-spinon  $s1$  fermions whose momentum values are good quantum numbers. For the Hubbard model on a square lattice in the one- and two-electron subspace the composite  $s1$  fermion consists of two spinons in a spin-singlet configuration plus an infinitely thin flux tube attached to it. Thus, each  $s1$  fermion appears to carry a fictitious magnetic solenoid with it as it moves around in the  $s1$  effective lattice. The square-lattice quantum liquid is further investigated in Refs.<sup>1,22</sup>.

Concerning previous studies on the large- $U$  Hubbard model and  $t - J$  model on a square lattice involving for instance the slave particle formalism<sup>6,34,35</sup> or Jordan-Wigner transformations<sup>21</sup>, the crucial requirement is to impose the single occupancy constraint. Here that constraint is naturally implemented for all values of  $U/4t > 0$ , since the spins associated with the spin  $SU(2)$  state representations refer to the rotated electrons of the singly occupied sites. Moreover, for the above schemes the spinless fermions arise from individual spins or spinons. In contrast, within the extended Jordan-Wigner transformation considered in this paper and Ref.<sup>1</sup> the  $s1$  fermions emerge from spin-neutral

two-spinon composite  $s1$  bond particles. Elsewhere the two-spinon occupancy configurations in the spin effective lattice of the  $s1$  bond particles are studied in detail for the model (1) in the one- and two-electron subspace<sup>18</sup>. This is a needed step for the investigations of Refs.<sup>1,22</sup> of the square-lattice quantum liquid of  $c$  and  $s1$  fermions with residual interactions. Following the results of these references, it is expected that such a quantum liquid captures the universal properties of general many-electron models with short-range interactions on the square lattice.

The general rotated-electron description introduced here for the Hubbard model on the square lattice is consistent with a ground state with long-range antiferromagnetic order for half filling, short-range incommensurate-spiral spin order for  $0 < x \ll 1$ , and short-range spin order for finite hole concentrations  $x$  below a  $U/4t$ -dependent critical value  $x_*$  above which the system is driven into a disordered state without short-range spin order. Strong evidence is given in Refs.<sup>22,32</sup> that for a well-defined hole-concentration range  $x \in (x_c, x_*)$  where  $x_c \approx 10^{-2}$  and  $x_* \in (0.23, 0.31)$  for approximately  $u_0 \leq U/4t \leq u_\pi$  a long-range superconducting order coexists with the short-range spin order in the square-lattice quantum liquid perturbed by small 3D anisotropy associated with weak plane coupling.

Finally, the results of Refs.<sup>1,22,32</sup> suggest that the description introduced in this paper is useful for the further understanding of the role played by the electronic correlations in the unusual properties of the hole-doped cuprates.

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### Appendix A: Full information about the quantum problem when defined in the LWS-subspace

In this Appendix we confirm that full information about the quantum problem can be achieved by defining it in the LWS-subspace spanned by the energy eigenstates that are both LWSs of the  $\eta$ -spin and spin algebras. By that we mean that all  $\mathcal{N}$ -electron operator matrix elements between energy eigenstates such that at least one of them is a non-LWS can be evaluated exactly in terms of a corresponding quantum problem involving another well-defined  $\mathcal{N}$ -electron operator acting onto the LWS-subspace. Here  $\mathcal{N} = 1, 2, \dots$  refers to one, two, or any other finite number of electrons so that the expression of the general  $\mathcal{N}$ -electron operator under consideration reduces to an elementary creation or annihilation electronic operator ( $\mathcal{N} = 1$ ) or involves the product of two or more such elementary operators ( $\mathcal{N} \geq 2$ ).

In addition, we show here that use of the model global symmetry provides a simple relation between the energy of any non-LWS and the corresponding LWS so that all contributions to the physical quantities from non-LWSs can be evaluated by considering a related problem defined in the LWS-subspace. The use of such a symmetry reveals that for hole concentration  $x > 0$  and spin density  $m > 0$  the ground state is always a LWS of both the  $\eta$ -spin and spin algebras. For simplicity here we consider matrix elements between the ground state and a non-LWS. Those appear in Lehmann representations of zero-temperature spectral functions and correlation functions, but similar results can be obtained for matrix elements between any excited energy eigenstates.

Expressions (8)-(11) for the  $c$  fermion,  $\eta$ -spinon, and spinon operators refer to the LWS-subspace. A similar representation can be used for instance for the HWS subspace, which is spanned by all energy eigenstates with  $S_\alpha = S_\alpha^z$  where  $\alpha = \eta, s$ . (There are also two mixed subspaces such that  $S_\eta = \pm S_\eta^z$  and  $S_s = \mp S_s^z$ .) The HWS representation is suitable for canonical ensembles referring to electronic densities larger than one and negative spin densities since then the ground states are HWSs of both the  $\eta$ -spin and spin algebras. The studies of this paper refer to the LWS-subspace. In this Appendix we provide the expressions for the  $c$  fermion,  $\eta$ -spinon, and spinon operators that are suitable for the HWS subspace.

#### 1. How to map the problem onto the LWS-subspace

We start by confirming that there is a well-defined  $\mathcal{N}$ -electron operator  $\hat{\Theta}_{\mathcal{N}}$  such that any matrix element  $\langle f | \hat{O}_{\mathcal{N}} | \psi_{GS} \rangle$  of a  $\mathcal{N}$ -electron operator  $\hat{O}_{\mathcal{N}}$  where  $|f\rangle$  is a non-LWS of the  $\eta$ -spin algebra and/or spin algebra and  $|\psi_{GS}\rangle$  the ground state of the Hubbard model on the 1D or square lattice can be written as  $\langle f | \hat{O}_{\mathcal{N}} | \psi_{GS} \rangle = \langle f.LWS | \hat{\Theta}_{\mathcal{N}} | \psi_{GS} \rangle$ . Here  $|f.LWS\rangle$  is the LWS that corresponds to the state  $|f\rangle$ . Within the two  $SU(2)$  algebras the latter state can be

expressed as,

$$|f\rangle = \prod_{\alpha=\eta, s} \frac{(\hat{S}_\alpha^\dagger)^{L_{\alpha, -1/2}}}{\sqrt{\mathcal{C}_\alpha}} |f.LWH\rangle, \quad (\text{A1})$$

where

$$\mathcal{C}_\alpha = \delta_{L_{\alpha, -1/2}, 0} + \prod_{l=1}^{L_{\alpha, -1/2}} l [L_\alpha + 1 - l], \quad (\text{A2})$$

is a normalization constant,  $L_{\alpha, -1/2} \leq L_\alpha = 2S_\alpha$ , and the  $\eta$ -spin flip ( $\alpha = \eta$ ) and spin flip ( $\alpha = s$ ) operators  $\hat{S}_\alpha^\dagger$  are the off-diagonal generators of the corresponding  $SU(2)$  algebras provided in Eq. (6). These operators remain invariant under the electron - rotated-electron unitary transformation and thus as given in that equation have the same expression in terms of electron and rotated-electron creation and annihilation operators.

As confirmed in Section IV, for a hole concentration  $x \geq 0$  and spin density  $m \geq 0$  the ground state is a LWS of both the  $\eta$ -spin and spin  $SU(2)$  algebras and thus has the following property,

$$\hat{S}_\alpha |\psi_{GS}\rangle = 0; \quad \alpha = \eta, s. \quad (\text{A3})$$

The operator  $\hat{\Theta}_\mathcal{N}$  is then such that,

$$\begin{aligned} \langle f | \hat{\Theta}_\mathcal{N} | \psi_{GS} \rangle &= \langle f.LWS | \prod_{\alpha=\eta, s} \frac{1}{\sqrt{\mathcal{C}_\alpha}} (\hat{S}_\alpha)^{L_{\alpha, -1/2}} \hat{\Theta}_\mathcal{N} | \psi_{GS} \rangle \\ &= \langle f.LHS | \hat{\Theta}_\mathcal{N} | \psi_{GS} \rangle. \end{aligned} \quad (\text{A4})$$

By the suitable use of Eq. (A3), it is straightforward to show that for  $L_{\eta, -1/2} > 0$  and/or  $L_{s, -1/2} > 0$  the operator  $\hat{\Theta}_\mathcal{N}$  is given by the following commutator,

$$\hat{\Theta}_\mathcal{N} = \left[ \prod_{\alpha=\eta, s} \frac{1}{\sqrt{\mathcal{C}_\alpha}} \right] \left[ \prod_{\alpha=\eta, s} (\hat{S}_\alpha)^{L_{\alpha, -1/2}}, \hat{O}_\mathcal{N} \right], \quad (\text{A5})$$

and by,

$$\hat{\Theta}_\mathcal{N} = \hat{O}_\mathcal{N}, \quad (\text{A6})$$

for  $L_{\eta, -1/2} = L_{s, -1/2} = 0$ . If the commutator on the right-hand side of Eq. (A5) vanishes then the matrix element  $\langle f | \hat{\Theta}_\mathcal{N} | \psi_{GS} \rangle$  under consideration also vanishes.

Let  $E_f$  denote the energy eigenvalue of the non-LWS  $|f\rangle$  and  $E_{f.LWS}$  that of the corresponding LWS  $|f.LWS\rangle$ . To find the relation between  $E_f$  and  $E_{f.LWS}$  one adds chemical-potential and magnetic-field operator terms to the Hamiltonian (1), what lowers its symmetry. Since our description refers to the LWS-subspace, we use units such that the sign of the chemical potential  $\mu \geq 0$  is that of the hole concentration  $x = [N_a^D - N]/N_a^D \geq 0$  and the sign of the magnetic field  $H \geq 0$  that of the spin density  $m = [N_\uparrow - N_\downarrow]/N_a^D \geq 0$ . Since such operator terms commute with the Hamiltonian (1), the rotated-electron occupancy configurations of all energy eigenstates correspond to state representations of its global symmetry for all densities. Moreover, the use of such commutation relations reveals that the energy eigenvalues  $E_f$  and  $E_{f.LWS}$  are related as,

$$E_f = E_{f.LWS} + \sum_{\alpha=\eta, s} \mu_\alpha L_{\alpha, -1/2}, \quad (\text{A7})$$

where  $\mu_\eta = 2\mu$  is twice the chemical potential whose range is  $2\mu^0 \leq 2\mu \leq U + 4Dt$  for  $D = 1, 2$ ,  $2\mu^0$  is the half-filling Mott-Hubbard gap considered in Subsection IV-C,  $\mu_s = 2\mu_B H \geq 0$ , and  $\mu_B$  is the Bohr magneton.

It follows from Eq. (A7) that  $E_f \geq E_{f.LWS}$ . For hole concentration  $x > 0$  and spin density  $m > 0$  such an inequality can be shown to be consistent with the ground state being always a LWS of both the  $\eta$ -spin and spin algebras. On the other hand, the model global symmetry requires that  $E_f = E_{f.LWS}$  for the half-filling and zero-magnetization absolute ground state. Such a requirement is fulfilled: for half filling one has that  $\mu \in (-\mu^0, \mu^0)$ . The value  $\mu = 0$  corresponds to the middle of the Mott-Hubbard gap, whereas the magnetic field  $H$  vanishes for zero magnetization. The absolute ground state corresponds to  $S_\eta = S_s = 0$  and  $S_c = N_a^D/2$  and hence is both a LWS and a HWS of the  $\eta$ -spin and spin algebras.

Within a Lehmann representation the  $\mathcal{N}$ -electron spectral functions are expressed as a sum of terms, one for each excited energy eigenstate. In spectral-function terms associated with non-LWSs one can then replace the matrix element  $\langle f | \hat{O}_{\mathcal{N}} | \psi_{GS} \rangle$  by  $\langle f | LHS | \hat{O}_{\mathcal{N}} | \psi_{GS} \rangle$  provided that the excited-state energy  $E_f$  is expressed as in Eq. (A7). Then the original  $\mathcal{N}$ -electron spectral function can be written as a sum of spectral functions of well-defined  $\mathcal{N}$ -electron operators of the form given in Eqs. (A5) or (A6), all acting onto the LWS-subspace.

These results confirm that full information about the present quantum problem can be obtained by defining it in the LWS-subspace.

## 2. Operators of the three elementary objects within the HWS representation

Within the HWS representation the  $c$  fermion operators read,

$$f_{\vec{r}_j, c}^\dagger = \tilde{c}_{\vec{r}_j, \downarrow}^\dagger (1 - \tilde{n}_{\vec{r}_j, \uparrow}) + e^{i\vec{\pi} \cdot \vec{r}_j} \tilde{c}_{\vec{r}_j, \downarrow} \tilde{n}_{\vec{r}_j, \uparrow}. \quad (\text{A8})$$

The  $\eta$ -spinon and spinon operators are given by Eq. (9) where now the operator  $n_{\vec{r}_j, c} = f_{\vec{r}_j, c}^\dagger f_{\vec{r}_j, c}$  of Eq. (10) involves the  $c$  fermion operator (A8) and the rotated quasi-spin operators  $q_{\vec{r}_j}^\pm = q_{\vec{r}_j}^x \pm i q_{\vec{r}_j}^y$  and  $q_{\vec{r}_j}^z$  read,

$$\begin{aligned} q_{\vec{r}_j}^+ &= \tilde{c}_{\vec{r}_j, \uparrow}^\dagger (\tilde{c}_{\vec{r}_j, \downarrow} - e^{i\vec{\pi} \cdot \vec{r}_j} \tilde{c}_{\vec{r}_j, \downarrow}^\dagger), \\ q_{\vec{r}_j}^- &= (q_{\vec{r}_j}^+)^\dagger; \quad q_{\vec{r}_j}^z = \tilde{n}_{\vec{r}_j, \downarrow} - \frac{1}{2}, \end{aligned} \quad (\text{A9})$$

respectively. After inverting such relations one finds that within the HWS representation the local rotated-electron operators can be expressed in terms of the local  $c$  fermion and rotated quasi-spin operators as follows,

$$\begin{aligned} \tilde{c}_{\vec{r}_j, \downarrow}^\dagger &= f_{\vec{r}_j, c}^\dagger \left( \frac{1}{2} - q_{\vec{r}_j}^z \right) + e^{i\vec{\pi} \cdot \vec{r}_j} f_{\vec{r}_j, c} \left( \frac{1}{2} + q_{\vec{r}_j}^z \right), \\ \tilde{c}_{\vec{r}_j, \uparrow}^\dagger &= q_{\vec{r}_j}^+ (f_{\vec{r}_j, c}^\dagger - e^{i\vec{\pi} \cdot \vec{r}_j} f_{\vec{r}_j, c}). \end{aligned} \quad (\text{A10})$$

The commutation and anti-commutation relations (12)-(16) are valid for all representations and hence are the same for both the LWS and HWS representations.

## Appendix B: Equivalence of the quantum numbers of the present description and those of the exact solution for 1D

### 1. Relation to the quantum numbers of the exact solution for $N_a \gg 1$

The studies of this paper establish that the spinons (and  $\eta$ -spinons) that are not invariant under the electron rotated-electron transformation are part of spin (and  $\eta$ -spin) neutral  $2\nu$ -spinon (and  $2\nu$ - $\eta$ -spinon) composite  $s\nu$  (and  $\eta\nu$ ) bond particles, which have a bounding (and an anti-bounding) character. Moreover, for the 1D model some neutral  $2\nu$ -spinon (and  $2\nu$ - $\eta$ -spinon) configurations exist that define suitable  $s\nu$  (and  $\eta\nu$ ) bond particles whose occupancies generate the energy eigenstates for  $U/4t > 0$ . The detailed structure of such configurations remains an open problem. It is studied in Ref.<sup>18</sup> both for the 1D and square lattices for the case of the one- and two-electron subspace as defined in this paper, where only the  $c$  fermions and  $s1$  bond particles have an active role.

By generalizing the procedures used in Ref.<sup>18</sup> for the  $s1$  bond particles to the remaining  $\alpha\nu$  bond-particle branches introduced in this paper, one finds that for the model on the 1D lattice such objects can be associated with  $\alpha\nu$  bond-particle operators  $g_{x_j, \alpha\nu}^\dagger$  of the general form,

$$g_{x_j, \alpha\nu} = \sum_g h_{\alpha\nu, g} a_{x_j, \alpha\nu, g}; \quad g_{x_j, \alpha\nu}^\dagger = (g_{x_j, \alpha\nu})^\dagger. \quad (\text{B1})$$

Here  $a_{x_j, \alpha\nu, g}$  is a superposition of operators belonging to a number of families, which increases for increasing values of the number  $\nu = 1, 2, \dots$  of spinon ( $\alpha = s$ ) or  $\eta$ -spinon ( $\alpha = \eta$ ) pairs, the spatial-coordinate  $x_j$  refers to the  $\alpha\nu$  effective lattice, the index  $j = 1, \dots, N_{\alpha\nu}$  to the sites of that lattice, and the index  $g$  to different types of  $2\nu$ -site links belonging to the same family as defined in that paper for the  $s1$  bond particles. The  $c$  effective lattice equals the original lattice and thus has length  $L = N_a a$  and lattice constant  $a$  so that  $x_j = j a$  for  $N_a \gg 1$ . The  $\alpha\nu$  effective



lattices have also length  $L$  yet the lattice constants read  $a_{\alpha\nu} = [N_a/N_{a_{\alpha\nu}}] a \geq a$  and are such that  $L = N_{a_{\alpha\nu}} a_{\alpha\nu}$  and  $x_j = j a_{\alpha\nu}$  where  $j = 1, \dots, N_{a_{\alpha\nu}}$ . Furthermore, according to the same results the number of sites of the  $\alpha\nu$  effective lattice  $N_{a_{\alpha\nu}}$  is for 1D given by expression (42) with  $D = 1$  so that  $N_{a_{\alpha\nu}} = N_{\alpha\nu} + N_{\alpha\nu}^h$  where  $N_{a_\alpha} \equiv N_{a_\alpha}^1$  and  $N_{\alpha\nu}$  is the number of composite  $\alpha\nu$  bond particles and hence of occupied sites of the  $\alpha\nu$  effective lattice. The corresponding number of unoccupied sites  $N_{\alpha\nu}^h$  of that lattice is provided in Eq. (43) with  $N_{a_\alpha}^D \equiv N_{a_{\alpha\nu}}$ . Here  $C_\alpha$  is the number of "occupied sites" of the  $\eta$ -spin ( $\alpha = \eta$ ) and spin ( $\alpha = s$ ) effective lattice, which refers to the subspaces with constant values of  $S_c$ ,  $S_\eta$ , and  $S_s$  and is given in Eq. (31) where  $N_{a_\alpha}^D \equiv N_{a_{\alpha\nu}}$  for 1D is the total number of sites of these effective lattices. Each subspace with constant values of  $S_c$  and hence also of  $N_{a_\eta} = [N_a - 2S_c]$  and  $N_{a_s} = 2S_c$  can be divided into smaller subspaces with constant values of  $S_c$ ,  $S_\eta$ , and  $S_s$  and hence also of  $C_\eta$  and  $C_s$ . Furthermore, the latter subspaces can be further divided into even smaller subspaces with constant values for the set of numbers  $\{N_{\eta\nu}\}$  and  $\{N_{s\nu}\}$ , which must obey the sum-rule of Eq. (31).

Concerning the operators  $a_{x_j, \alpha\nu, g}$  of the general expressions given in Eq. (B1), the simplest case refers to the  $s1$  bond particles whose number of families is two and for instance for the  $N_{s1}^h = 0$  configuration state the operator  $a_{x_j, s1, g}$  is given by<sup>18</sup>,

$$a_{x_j, s1, g} = \sum_{l=\pm 1} b_{x_j + \vec{r}_{1,l}^0, s1, l, g}; \quad b_{x, s1, l, g}^\dagger = \frac{1}{\sqrt{2}} \left( \left[ \frac{1}{2} + s_{x-x_l}^z \right] s_{x+x_l}^- - \left[ \frac{1}{2} + s_{x+x_l}^z \right] s_{x-x_l}^- \right), \quad (\text{B2})$$

and  $b_{x, s1, l, g} = (b_{x, s1, l, g}^\dagger)^\dagger$ . Here the spinon operators are given in Eq. (9) and for simplicity we have omitted the family index  $d$ , which reads  $d = 1$  for 1D so that  $x_l$  corresponds to the general two-site link vector  $\vec{r}_{d,l}$  introduced in Ref.<sup>18</sup>.

The studies of Ref.<sup>18</sup> lead to  $s1$  bond-particle operators that are shown in that paper to obey a hard-core algebra. For 1D it follows straightforwardly that the two- $\eta$ -spinons  $\eta1$  bond-particle operators also obey such an algebra. One then considers the four-spinon  $s2$  bond-particle and four- $\eta$ -spinon  $\eta2$  bond-particle operator problems and finds that operators of the general form (B1) can be constructed by procedures similar to those used for the  $s1$  and  $\eta1$  bond-particle operators so that the hard-core algebra is obeyed.

We skip here the details of such derivations since the basic procedures are the same as those already used for the two-spinon  $s1$  bond particles in Ref.<sup>18</sup> except that the algebraic manipulations are for  $\nu > 1$  much more cumbersome. Moreover, it turns out that for interesting applications within the dynamical theory of Ref.<sup>53</sup> referring to the model on the 1D lattice, such as the evaluation for finite excitation energy  $\omega$  of one- and two-electron matrix elements between the ground state and excited states and corresponding spectral-weight distributions, only excited states involving  $c$  and  $s1$  fermions and a finite number of  $s\nu$  fermions with  $\nu > 1$  spinon pairs lead to finite spectral weight. The latter  $s\nu$  fermions have vanishing energy and momentum and remain invariant under the electron - rotated-electron unitary transformation so that the only effect of their creation and annihilation is in the numbers of  $s1$  fermions and  $s1$  band discrete momentum values. Therefore, for the excited states contributing to the dynamical theory of Ref.<sup>53</sup> only the  $c$  fermions and  $s1$  fermions play an active role.

The only general result this is needed for the goals of this Appendix is that alike for the two-site one-bond operators, composite  $\alpha\nu$  bond-particle operators of general form given in Eq. (B1) can for 1D be constructed so that when acting onto the LWS Hilbert space they anticommute on the same  $\alpha\nu$  effective-lattice site,

$$\{g_{x_j, \alpha\nu}^\dagger, g_{x_j, \alpha\nu}\} = 1; \quad \{g_{x_j, \alpha\nu}^\dagger, g_{x_j, \alpha\nu}^\dagger\} = \{g_{x_j, \alpha\nu}, g_{x_j, \alpha\nu}\} = 0, \quad (\text{B3})$$

and commute on different sites,

$$[g_{x_j, \alpha\nu}^\dagger, g_{x_{j'}, \alpha\nu}] = [g_{x_j, \alpha\nu}^\dagger, g_{x_{j'}, \alpha\nu}^\dagger] = [g_{x_j, \alpha\nu}, g_{x_{j'}, \alpha\nu}] = 0; \quad j \neq j'. \quad (\text{B4})$$

Furthermore, such operators commute with the  $c$  fermion operators and operators corresponding to different  $\alpha\nu$  branches also commute with each other.

In this Appendix we confirm that the general hard-core algebra of Eqs. (B3) and (B4) combined with the universal number expressions given in Section IV leads to discrete momentum values for the  $c$  and  $\alpha\nu$  fermions that coincide with the quantum numbers of the exact solution for the whole LWS Hilbert subspace it refers to.

It follows from such an algebra that one can perform an extended Jordan-Wigner transformation that transforms the  $\alpha\nu$  bond particles into  $\alpha\nu$  fermions with operators  $f_{x_j, \alpha\nu}^\dagger$ . Alike in the general expressions provided in Eq. (24), such operators are related to the corresponding bond-particle operators as,

$$f_{x_j, \alpha\nu}^\dagger = e^{i\phi_{j, \alpha\nu}} g_{x_j, \alpha\nu}^\dagger; \quad f_{x_j, \alpha\nu} = e^{-i\phi_{j, \alpha\nu}} g_{x_j, \alpha\nu}, \quad (\text{B5})$$

where

$$\phi_{j, \alpha\nu} = \sum_{j' \neq j} f_{x_{j'}, \alpha\nu}^\dagger f_{x_{j'}, \alpha\nu} \phi_{j', j, \alpha\nu}; \quad \phi_{j', j, \alpha\nu} = \arctan \left( \frac{y_{j'} - y_j}{x_{j'} - x_j} \right); \quad 0 \leq \phi_{j', j, \alpha\nu} \leq 2\pi. \quad (\text{B6})$$

However, for 1D the coordinate  $z_j = x_j + i y_j$  is such that  $y_j = 0$  and hence reduces to the real-space coordinate  $x_j$  of the  $\alpha\nu$  bond particle in its  $\alpha\nu$  effective lattice. Therefore, for 1D the phase  $\phi_{j',j,\alpha\nu}$  can for all  $\alpha\nu$  branches have the values  $\phi_{j',j,\alpha\nu} = 0$  and  $\phi_{j',j,\alpha\nu} = \pi$  only. Indeed, the relative angle between two sites of the  $\alpha\nu$  effective lattice in a 1D chain can only be one of the two values. Then the  $\alpha\nu$  phase factor of Eq. (B6) is such that,

$$e^{ia_{\alpha\nu} \frac{\partial}{\partial x} \phi_{\alpha\nu}(x)|_{x=x_j}} = e^{i(\phi_{j+1,\alpha\nu} - \phi_{j,\alpha\nu})} = e^{i\pi f_{x_j,\alpha\nu}^\dagger f_{x_j,\alpha\nu}}, \quad (\text{B7})$$

where  $\phi_{\alpha\nu}(x_j) \equiv \phi_{j,\alpha\nu}$ .

The  $c$  fermion operators have the anticommuting relations given in Eq. (12), which for 1D read,

$$\{f_{x_j,c}^\dagger, f_{x_{j'},c}\} = \delta_{j,j'}; \quad \{f_{x_j,c}^\dagger, f_{x_{j'},c}^\dagger\} = \{f_{x_j,c}, f_{x_{j'},c}\} = 0. \quad (\text{B8})$$

Moreover, the  $\alpha\nu$  bond-particle operators that emerge from the Jordan-Wigner transformation associated with Eqs. (B5) and (B6) have similar anticommuting relations given by,

$$\{f_{x_j,\alpha\nu}^\dagger, f_{x_{j'},\alpha\nu}\} = \delta_{j,j'}; \quad \{f_{x_j,\alpha\nu}^\dagger, f_{x_{j'},\alpha\nu}^\dagger\} = \{f_{x_j,\alpha\nu}, f_{x_{j'},\alpha\nu}\} = 0, \quad (\text{B9})$$

and the  $c$  fermion operators commute with the  $\alpha\nu$  fermion operators and  $\alpha\nu$  and  $\alpha'\nu'$  fermion operators such that  $\alpha\nu \neq \alpha'\nu'$  also commute.

One can introduce  $c$  fermion operators given in Eq. (8) associated with discrete momentum values, which for 1D read,

$$f_{q_j,c}^\dagger = \frac{1}{\sqrt{N_a}} \sum_{j'=1}^{N_a} e^{+iq_j x_{j'}} f_{x_{j'},c}^\dagger; \quad f_{q_j,c} = \frac{1}{\sqrt{N_a}} \sum_{j'=1}^{N_a} e^{-iq_j x_{j'}} f_{x_{j'},c}; \quad j = 1, \dots, N_a; \quad x_j = ja; \quad L = aN_a. \quad (\text{B10})$$

For the 1D Hubbard model the  $\alpha\nu$  fermion operators  $f_{q_j,\alpha\nu}^\dagger$  given in Eq. (24) labeled by the discrete momentum values  $q_j$  such that  $j = 1, \dots, N_{a_{\alpha\nu}}$ , which are the conjugate variables of the  $\alpha\nu$  effective lattice spatial coordinates  $x_j$ , can be introduced provided that the ratio  $N_{a_{\alpha\nu}}/N_a$  involving the number  $N_{a_{\alpha\nu}}$  of sites of the  $\alpha\nu$  effective lattice given in Eqs. (42) and (43) is finite for  $N_a \rightarrow \infty$ ,

$$f_{q_j,\alpha\nu}^\dagger = \frac{1}{\sqrt{N_{a_{\alpha\nu}}}} \sum_{j'=1}^{N_{a_{\alpha\nu}}} e^{+iq_j x_{j'}} f_{x_{j'},\alpha\nu}^\dagger; \quad f_{q_j,\alpha\nu} = \frac{1}{\sqrt{N_{a_{\alpha\nu}}}} \sum_{j'=1}^{N_{a_{\alpha\nu}}} e^{-iq_j x_{j'}} f_{x_{j'},\alpha\nu}; \quad j = 1, \dots, N_{a_{\alpha\nu}}; \quad x_j = ja_{\alpha\nu}, \quad (\text{B11})$$

where  $L = a_{\alpha\nu} N_{a_{\alpha\nu}}$ .

In 1D the phase factor  $e^{i\phi_{j,\alpha\nu}}$  does not have any effect when operating before  $f_{x_j,\alpha\nu}^\dagger$ . It follows that in 1D the expression of the Hamiltonian does not involve the phase  $\phi_{j,\alpha\nu}$ . Moreover, expression of the 1D normal-ordered Hamiltonian in terms of the  $c$  and  $\alpha\nu$  fermion operators reveals that such objects have zero-momentum forward-scattering only. This is consistent with the integrability of the model in 1D and the existence of an infinite number of conservations laws for the limit  $N_a \rightarrow \infty$  that our description refers to<sup>16</sup>. For the 1D model the occurrence of such conservations laws is behind the set of  $\alpha\nu$  fermion numbers  $\{N_{\alpha\nu}\}$  being good quantum numbers<sup>46</sup>. This is in contrast to the model on the square lattice, for which such numbers are not in general conserved, yet the quantity  $C_\alpha = \sum_\nu \nu N_{\alpha\nu}$  is.

The Jordan-Wigner transformations phases  $\phi_{j,\alpha\nu}$  have direct effects on the boundary conditions, which determine the discrete momentum values  $q_j$  of both the  $c$  and  $\alpha\nu$  fermion operators of Eqs. (B10) and (B11), respectively. In 1D the periodic boundary conditions of the original electron problem are ensured provided that one takes into account the effects of the Jordan-Wigner transformation on the boundary conditions of the  $c$  fermions and  $\alpha\nu$  fermions upon moving one of such objects around the chain of length  $L$  once.

As discussed in Subsection IV-B, for both the model on the 1D and square lattices the rotated-electron occupancies of the sites of the original lattice separate into two degrees of freedom only. (In the remaining of this Appendix we limit our considerations to the 1D problem.) Those of the  $2S_c$  sites of the original lattice singly occupied by rotated electrons separate into (i)  $2S_c$  sites of the  $c$  effective lattice occupied by  $c$  fermions and (ii)  $2S_c$  sites of the spin effective lattice occupied by spinons. Those of the  $[N_a - 2S_c]$  sites of the original lattice doubly occupied and unoccupied by rotated electrons separate into (i)  $[N_a - 2S_c]$  sites of the  $c$  effective lattice unoccupied by  $c$  fermions and (ii)  $[N_a - 2S_c]$  sites of the  $\eta$ -spin effective lattice occupied by  $\eta$ -spinons.

For instance, the  $2\nu$  sites of the spin (and  $\eta$ -spin) effective lattice referring to the occupancy configuration of one local  $2\nu$ -spinon composite  $s\nu$  fermion (and  $2\nu$ - $\eta$ -spinon composite  $\eta\nu$  fermion) correspond to the spin (and  $\eta$ -spin) degrees of freedom of  $2\nu$  sites of the original lattice whose degrees of freedom associated with the global  $U(1)$  symmetry found in Ref.<sup>2</sup> are described by  $2\nu$  sites of the  $c$  effective lattice occupied (and unoccupied) by  $c$  fermions.

An important point is that the independent spinons and independent  $\eta$ -spinons are not part of the Jordan-Wigner transformations that transform the  $\alpha\nu$  bond particles onto  $\alpha\nu$  fermions. It follows that when one  $c$  fermion moves around its effective lattice of length  $L$  it feels the effects of the Jordan-Wigner transformations through the sites of the spin and  $\eta$ -spin lattices associated with those of the  $s\nu$  and  $\eta\nu$  effective lattices occupied by  $s\nu$  and  $\eta\nu$  fermions, respectively. Indeed, we recall that the sites of the  $c$  effective lattice on the one hand and those of the spin and  $\eta$ -spin effective lattices on the other hand correspond to the different degrees of freedom of rotated-electron occupancies of the same sites of the original lattice.

Since the  $c$  fermions do not emerge from a Jordan-Wigner transformation and each  $\alpha\nu$  fermion corresponds to a set of  $2\nu$  sites of the original lattice different from and independent of those of any other  $\alpha'\nu'$  fermion, when a  $\alpha\nu$  fermion moves around its  $\alpha\nu$  effective lattice of length  $L$  it only feels the Jordan-Wigner-transformation phases of its own lattice associated with both the  $\alpha\nu$  fermions and  $\alpha\nu$  fermion holes so that its discrete momentum values obey the following periodic or anti-periodic boundary conditions,

$$e^{iq_j L} = \prod_{j=1}^{N_{a_{\alpha\nu}}} \left\{ \left[ e^{i(\phi_{j+1,\alpha\nu} - \phi_{j,\alpha\nu})} \right]^\dagger e^{i(\phi_{j+1,\alpha\nu} - \phi_{j,\alpha\nu})} \right\} = e^{i\pi[N_{a_{\alpha\nu}} - 1]} = -e^{i\pi N_{a_{\alpha\nu}}} . \quad (\text{B12})$$

Here the phase factor reads 1 and  $-1$  for  $[N_{a_{\alpha\nu}} - 1]$  even and odd, respectively. The term  $-1$  in  $[N_{a_{\alpha\nu}} - 1]$  can be understood as referring to the site occupied by the  $\alpha\nu$  fermion moving around its effective lattice and must be excluded. For the  $\alpha\nu$  fermions the unoccupied sites of their  $\alpha\nu$  effective lattice exist in their own right. Indeed, note that according to Eq. (B5) both the creation and annihilation operators of such objects involve the Jordan-Wigner-transformation phase  $\phi_{j,\alpha\nu}$ . As a result such a phase affects both the  $\alpha\nu$  fermions and  $\alpha\nu$  fermion holes. That justifies why the phase factor  $e^{i\pi[N_{a_{\alpha\nu}} - 1]}$  of Eq. (B12) involves all the  $N_{a_{\alpha\nu}} = [N_{\alpha\nu} + N_{\alpha\nu}^h]$  sites of the  $\alpha\nu$  effective lattice except that occupied by the moving  $\alpha\nu$  fermion. Hence it involves both the  $[N_{\alpha\nu} - 1]$  sites occupied by the remaining fermions of the same  $\alpha\nu$  branch and the corresponding  $N_{\alpha\nu}^h$   $\alpha\nu$  fermion holes.

In contrast, the  $c$  fermions are affected by the sites occupied by  $\alpha\nu$  fermions only. Indeed, only the sets of  $2\nu$  sites of the spin (and  $\eta$ -spin) effective lattice associated with each occupied site of the  $s\nu$  (and  $\eta\nu$ )  $\nu = 1, 2, 3, \dots$  effective lattices and the sites of the spin (and  $\eta$ -spin) effective lattice occupied by independent spinons (and independent  $\eta$ -spinons) correspond to sites of the original lattice whose degrees of freedom associated with the  $c$  fermion  $U(1)$  symmetry are described by the occupancy configurations of the  $c$  effective lattice. However, the independent spinons (and independent  $\eta$ -spinons) do not undergo any Jordan-Wigner transformation so that due to the Jordan-Wigner-transformation phase  $\phi_{j',\alpha\nu}$  of each of the  $N_{\alpha\nu}$   $\alpha\nu$  fermions at sites  $j' = 1, \dots, N_{\alpha\nu}$  of their  $\alpha\nu$  effective lattice the  $c$  fermion discrete momentum values are determined by the following periodic or anti-periodic boundary condition,

$$e^{iq_j L} = \prod_{\alpha\nu} \prod_{j'=1}^{N_{\alpha\nu}} e^{i(\phi_{j'+1,\alpha\nu} - \phi_{j',\alpha\nu})} = e^{i\pi \sum_{\alpha\nu} N_{\alpha\nu}} . \quad (\text{B13})$$

Again the phase factor on the right-hand side of Eq. (B13) reads 1 and  $-1$  for  $\sum_{\alpha\nu} N_{\alpha\nu}$  even and odd, respectively.

The above results imply that the discrete momentum values  $q_j$  of both  $c$  and  $\alpha\nu$  fermions have the usual momentum spacing  $q_{j+1} - q_j = 2\pi/L$  and read,

$$q_j = \frac{2\pi}{L} I_j^{\alpha\nu} ; \quad j = 1, \dots, N_{a_{\alpha\nu}} ; \quad q_j = \frac{2\pi}{L} I_j^c ; \quad j = 1, \dots, N_a . \quad (\text{B14})$$

However, following the boundary conditions (B12) [and (B13)] the numbers  $I_j^{\alpha\nu}$  (and  $I_j^c$ ) where  $j = 1, 2, \dots, N_{a_{\alpha\nu}}$  (and  $j = 1, 2, \dots, N_a$ ) appearing in this equation are not always integers. They are integers and half-odd integers for  $[N_{a_{\alpha\nu}} - 1]$  (and  $\sum_{\alpha\nu} N_{\alpha\nu}$ ) even and odd, respectively. Furthermore, as a result of the periodic or anti-periodic character of such boundary conditions these numbers obey the inequality  $|I_j^{\alpha\nu}| \leq [N_{a_{\alpha\nu}} - 1]/2$  for both  $[N_{a_{\alpha\nu}} - 1]$  odd and even (and the inequality  $|I_j^c| \leq [N_a - 1]/2$  for  $\sum_{\alpha\nu} N_{\alpha\nu}$  even and  $-[N_a - 2]/2 \leq I_j^c \leq N_a/2$  for  $\sum_{\alpha\nu} N_{\alpha\nu}$  odd).

For the one- and two-electron subspace one can separate the numbers  $I_j^{s1}$  and  $I_j^c$  of Eq. (B14) in two terms corresponding to an integer number and a small deviation as  $I_j^{s1} \equiv [\mathcal{N}_j^{s1} + \frac{q_{s1}^0}{2\pi} \frac{L}{N_{s1}}]$  and  $I_j^c \equiv [\mathcal{N}_j^c + \frac{q_c^0}{2\pi} \frac{L}{N_c}]$ , respectively. The corresponding  $c$  and  $s1$  fermion discrete momentum values then read,

$$\begin{aligned} q_j &= \frac{2\pi}{L} \mathcal{N}_j^c + q_c^0/N_c ; \quad \mathcal{N}_j^c = j - \frac{N_a}{2} = 0, \pm 1, \pm 2, \dots ; \quad j = 1, \dots, N_a . \\ q_j &= \frac{2\pi}{L} \mathcal{N}_j^{s1} + q_{s1}^0/N_{s1} ; \quad \mathcal{N}_j^{s1} = j - \frac{N_{a_{s1}}}{2} = 0, \pm 1, \pm 2, \dots ; \quad j = 1, \dots, N_{a_{s1}} , \end{aligned} \quad (\text{B15})$$

Here  $q_c^0$  (and  $q_{s1}^0$ ) is given either by  $q_c^0 = 0$  or  $q_c^0 = \pi[N_c/L]$  (and  $q_{s1}^0 = 0$  or  $q_{s1}^0 = \pi[N_{s1}/L]$ ) for all  $j = 1, \dots, N_a$  (and  $j = 1, \dots, N_{a_{s1}}$ ) discrete momentum values of the  $c$  (and  $s1$ ) band whose momentum occupancy describes a given state and the  $s1$  effective lattice length  $L = N_{a_{s1}} a_{s1}$  where  $a_{s1} = L/N_{a_{s1}} = [N_a/N_{a_{s1}}] a$  is the  $s1$  effective lattice constant.

Importantly, the  $c$  fermion and  $\alpha\nu$  fermion discrete momentum values obtained from our  $N_a \gg 1$  operational description of the quantum problem correspond to the Bethe-ansatz quantum numbers of the exact solution. Indeed, the discrete momentum values of Eq. (B14) can be expressed as,

$$q_j = \frac{2\pi}{L} I_j; \quad j = 1, \dots, N_a; \quad q_j = \frac{2\pi}{L} J_j^{\nu}; \quad j = 1, \dots, N_{a_{\eta\nu}}; \quad q_j = \frac{2\pi}{L} J_j^{\nu}; \quad j = 1, \dots, N_{a_{s\nu}}, \quad (\text{B16})$$

where  $I_j \equiv I_j^c$ ,  $J_j^{\nu} \equiv I_j^{\eta\nu}$ , and  $J_j^{\nu} \equiv I_j^{s\nu}$  are the exact-solution integers or half integers quantum numbers involved in Eqs. (2.12a)-(2.12c) of Ref.<sup>17</sup> and defined in the unnumbered equations provided below these equations (in the notation of that reference  $\nu = n$  and  $j = \alpha$  in  $J_j^{\nu}$  and  $J_j^{\nu}$ ). Moreover, the numbers on the right-hand side of the two inequalities given just above Eq. (2.13a) of that reference correspond to  $N_{a_{\eta\nu}}/2$  and  $N_{a_{s\nu}}/2$ , respectively, so that these inequalities read  $|J_j^{\nu}| < N_{a_{\eta\nu}}/2$  and  $|J_j^{\nu}| < N_{a_{s\nu}}/2$ . That is fully consistent with the above inequality  $|I_j^{\alpha\nu}| \leq [N_{a_{\alpha\nu}} - 1]/2$  where  $\alpha = \eta, s$  and  $N_{a_{\alpha\nu}}$  is given in Eq. (42). A careful comparison of the notations and definitions used in Ref.<sup>17</sup> and here confirms that there is also full consistency between the even or odd character of the integer numbers  $[N_{a_{\eta\nu}} - 1]$ ,  $[N_{a_{s\nu}} - 1]$ , and  $\sum_{\alpha\nu} N_{\alpha\nu}$  considered here and those that determine the integer of half-integer character of the quantum numbers  $J_j^{\nu} \equiv I_j^{\eta\nu}$ ,  $J_j^{\nu} \equiv I_j^{s\nu}$ , and  $I_j \equiv I_j^c$ , respectively, in that reference.

We emphasize that for the  $\alpha\nu$  fermions the discrete momentum values  $q_j$  of Eq. (B16) are the eigenvalues of the translation generator in the presence of the fictitious magnetic field of Eq. (25), which for 1D reads  $\vec{B}_{\alpha\nu}(x_j) = \sum_{j' \neq j} n_{x_{j'}, \alpha\nu} \delta(x_{j'} - x_j) \vec{e}_{x_3}$ . Hence the corresponding exact-solution quantum numbers are the eigenvalues of such a translator operator in units of  $2\pi/L$ .

Since for 1D the numbers  $\{N_{\alpha\nu}\}$  of  $\alpha\nu$  fermions are conserved, that the discrete momentum values  $q_j$  of the  $c$  and  $\alpha\nu$  fermions are good quantum numbers is consistent with the momentum operator commuting with the unitary operator  $\hat{V}^\dagger$  as defined in this paper. That operator generates exact  $U/4t > 0$  energy and momentum eigenstates  $|\Psi_{LWS;U/4t}\rangle = \hat{V}^\dagger |\Psi_{LWS;\infty}\rangle$  of general form given in Eq. (60) where in 1D  $|\Psi_{LWS;U/4t}\rangle = |\Phi_{LWS;U/4t}\rangle$  with  $U/4t$ -dependent energy eigenvalues but  $U/4t$ -independent momentum eigenvalues from the  $U/4t \rightarrow \infty$  energy and momentum eigenstates  $|\Psi_{LWS;\infty}\rangle$  of Eq. (58). Hence the momentum eigenvalues are fully determined by the  $U/4t \gg 1$  physics.

The use of the exact solution of the 1D problem confirms that the momentum eigenvalues have the general form given in Eq. (63). For 1D they may be written as,

$$P = \sum_{j=1}^{N_a} q_j N_c(q_j) + \sum_{\nu} \sum_{j'=1}^{N_{a_{s\nu}}} q_{j'} N_{s\nu}(q_{j'}) + \sum_{\eta\nu} \sum_{j'=1}^{N_{a_{\eta\nu}}} [\pi - q_{j'}] N_{\eta\nu}(q_{j'}) + \pi M_{\eta, -1/2}. \quad (\text{B17})$$

Here  $M_{\eta, -1/2}$  is the total number of  $\eta$ -spin-projection  $-1/2$   $\eta$ -spinons and the distributions  $N_c(q_j)$  and  $N_{\alpha\nu}(q_{j'})$  are the eigenvalues of the operators  $\hat{N}_c(q_j) = f_{q_j, c}^\dagger f_{q_j, c}$  and  $\hat{N}_{\alpha\nu}(q_j) = f_{q_j, \alpha\nu}^\dagger f_{q_j, \alpha\nu}$ , respectively, which have values 1 and 0 for occupied and unoccupied momentum values, respectively. One may obtain expression (B17) from analysis of the 1D problem for  $U/4t \gg 1$  without the use of Bethe ansatz, whose starting point is that for  $U/t \rightarrow \infty$  the electrons that singly occupy sites do not feel the on-site repulsion. Consistently, expression (B17) is that also provided by the exact solution after the rapidities are replaced by the quantum numbers  $I_j \equiv I_j^c$ ,  $J_j^{\nu} \equiv I_j^{\eta\nu}$ , and  $J_j^{\nu} \equiv I_j^{s\nu}$  related to the discrete momentum values  $q_j$  by Eq. (B16).

That the physical momentum (B17) is for  $U/4t > 0$  additive in the  $c$  and  $\alpha\nu$  fermion discrete momentum values follows from the latter being good quantum numbers whose occupancy configurations generate the energy eigenstates. It follows from the direct relation to the thermodynamic Bethe ansatz equations of Ref.<sup>17</sup> that the  $c$  fermions obtained here from the rotated electrons through Eq. (8) and the  $\alpha\nu$  fermions that emerge from the Jordan-Wigner transformations of Eq. (B5) are for the 1D lattice the  $c$  pseudoparticles and  $\alpha\nu$  pseudoparticles, respectively, associated in Ref.<sup>37</sup> with the Bethe-ansatz quantum numbers. The momentum quantum numbers of Eq. (B16) are precisely those given in Eq. (A.1) of Ref.<sup>37</sup> and the numbers  $N_{a_{\alpha\nu}}$  of Eq. (42) equal the numbers  $N_{\alpha\nu}^*$  defined by its Eqs. (B.6), (B.7), and (B.11) with the index  $c$  replaced by  $\eta$ . Furthermore, the  $\eta$ -spinons and spinons considered here are for 1D the holons and spinons of that reference, respectively. Also the independent  $\eta$ -spinons and independent spinons are for 1D the Yang holons and HL spinons, respectively, of Ref.<sup>37</sup>. (In the notation of that reference HL stands for Heilmann and Lieb.)

## 2. Relation to the algebraic formulation of the exact solution

We just confirmed that for 1D the discrete momentum values of the  $c$  fermion operators  $f_{q_j, c}^\dagger$ , which within our description emerge from the electron - rotated-electron unitary transformation, and those of the  $\alpha\nu$  fermion operators

$f_{qj,\alpha\nu}^\dagger$ , which emerge from that transformation and an extended Jordan-Wigner transformation, equal the quantum numbers of the exact Bethe-ansatz solution. Such a result was obtained in the limit  $N_a \gg 1$  that the description considered in this paper and in Refs.<sup>1,18</sup> refers to. However, such a connection corresponds to the quantum numbers only and the relation of the  $c$  and  $\alpha\nu$  fermion operators to the exact solution of the 1D model remains an open problem.

The relation of the building blocks of our description to the original electrons is uniquely defined yet corresponds to a complex problem. Such building blocks are the  $c$  fermions,  $\eta$ -spinons, and spinons. For  $U/4t \gg 1$  the rotated electrons become electrons and the  $c$  fermion creation operator  $f_{\vec{r}j,c}^\dagger$  becomes the quasicharge annihilation operator  $\hat{c}_r$  of Ref.<sup>12</sup>. Therefore, in that limit the  $c$  fermions are the "holes" of the quasicharge particles of that reference whereas the spinons and  $\eta$ -spinons are associated with the local spin and pseudospin operators, respectively, of the same reference. The transformation considered in Ref.<sup>12</sup> does not introduce Hilbert-space constraints. It follows that suitable occupancy configurations of the objects associated with the local quasicharge, spin, and pseudospin operators considered in that reference exist that generate a complete set of states. However, only in the limit  $U/4t \gg 1$  suitable occupancy configurations of such basic objects generate exact energy eigenstates.

The point is that rotated electrons as defined in this paper are related to electrons by a unitary transformation. And such a transformation is such that for  $U/4t > 0$  rotated-electron occupancy configurations of the same form as those that generate energy eigenstates for  $U/4t \gg 1$  in terms of electron operators do generate energy eigenstates for finite values of  $U/4t$ . The  $c$  fermion,  $\eta$ -spinon, and spinon operators are related to the rotated-electron operators as the quasicharge, spin, and pseudospin operators of Ref.<sup>12</sup> are related to electron operators.

Importantly, note that the validity of the  $c$  fermion, spinon, and  $\eta$ -spinon operational description constructed in this paper and in Refs.<sup>1,18</sup> for the Hubbard model on a square and 1D lattices is for the 1D problem independent of its relation to the exact solution. For the LWS subspace that such a solution refers to the validity of our operational description follows from the transformations behind it not introducing Hilbert-space constraints. Such a transformations correspond to explicit operator expressions in terms of rotated-electron operators: For the  $c$  fermion operators such an expression is given in Eq. (8) and for the spinon and  $\eta$ -spinon operators in Eqs. (9)-(11). And the rotated-electron operators are related to the original electron operators by the unitary transformation  $\tilde{c}_{\vec{r}j,\sigma}^\dagger = \hat{V}^\dagger c_{\vec{r}j,\sigma}^\dagger \hat{V}$  whose unitary operator  $\hat{V}^\dagger$  is within our description uniquely defined. For  $U/4t > 0$  it has been constructed to inherently generating a complete set of energy eigenstates of the general form  $|\Psi_{LWS;U/4t}\rangle = \hat{V}^\dagger |\Psi_{LWS;\infty}\rangle$  with  $\{|\Psi_{LWS;\infty}\rangle\}$  being a complete set of suitably chosen  $U/4t \gg 1$  energy eigenstates. For 1D such states are such that  $|\Psi_{LWS;U/4t}\rangle = |\Phi_{LWS;U/4t}\rangle$  where  $|\Phi_{LWS;U/4t}\rangle = \hat{V}^\dagger |\Phi_{LWS;\infty}\rangle$  are the states of general form given in Eq. (60).

In order to clarify the relation of the  $c$  and  $\alpha\nu$  fermion operators to the exact solution of the 1D model rather than the so called coordinate Bethe ansatz<sup>15,17</sup> it is convenient to consider the solution of the problem by an algebraic operator formulation where the HWSs or LWSs of the  $\eta$ -spin and spin algebras are built up in terms of linear combination of products of several types of creation fields acting onto the hole or electronic vacuum, respectively<sup>16,24</sup>. The model energy eigenstates that are HWSs or LWSs of these algebras are often called *Bethe states*. Here we briefly discuss how in 1D and for  $N_a \gg 1$  the  $c$  and  $\alpha\nu$  fermion operators emerge from the creation fields of the algebraic formulation of the Bethe states.

That the general description introduced in this paper for the Hubbard model on the square and 1D lattices is consistent with the exact solution of the 1D problem at the operator level as well confirms its validity for 1D and this is the only motivation and aim of this Appendix. However, since that refers to a side problem of the square-lattice quantum liquid of  $c$  and  $s1$  fermions studied in this paper, in the following discussion we skip most technical details that are unnecessary for its general goals. Nevertheless provided that our analysis of the problem is complemented with the detailed information provided in Refs.<sup>16,17</sup> the resulting message clarifies the main issues under consideration.

The algebraic formulation of the Bethe states refers to the transfer matrix of the classical coupled spin model, which is the "covering" 1D Hubbard model<sup>54</sup>. Indeed, within the inverse scattering method<sup>16</sup> the central object to be diagonalized is the quantum transfer matrix rather than the underlying 1D Hubbard model. The transfer-matrix eigenvalues provide the spectrum of a set of  $[N_a - 1]$  conserved charges. The creation and annihilation fields are labeled by the Bethe-ansatz rapidities  $\lambda$ , which may be generally complex and are not the ultimate quantum numbers of the model. Many quantities are functions of such rapidities. For instance, the weights  $a(\lambda)$  and  $b(\lambda)$  considered in the derivation of Ref.<sup>16</sup> satisfy the free-fermion condition  $a(\lambda)^2 + b(\lambda)^2 = 1$ . (A possible and often used parametrization is  $a(\lambda) = \cos(\lambda)$  and  $b(\lambda) = \sin(\lambda)$ .) The reparametrization  $\tilde{\lambda} = [a(\lambda)/b(\lambda)] e^{2h(\lambda)} - [b(\lambda)/a(\lambda)] e^{-2h(\lambda)} - U/2$  where the constraint  $h(\lambda)$  is defined by the relation  $\sinh[2h(\lambda)] = [U/2] a(\lambda)b(\lambda)$ , plays an important role in the derivation in the context of the quantum inverse scattering method of the non-trivial Boltzmann weights of the isotropic six-vertex model given in Eq. (33) of Ref.<sup>16</sup>.

The diagonalization of the charge degrees of freedom involves a transfer matrix of the form provided in Eq. (21) of that reference, whose off-diagonal entries are some of the above mentioned creation and annihilation fields. The commutation relations of such important operators play a major role in the theory and are given in Eqs. (25), (40)-

(42), (B.1)-(B.3), (B.7)-(B.11), and (B.19)-(B.22) of the same reference. The solution of the spin degrees of freedom involves the diagonalization of the auxiliary transfer matrix associated with the monodromy matrix provided in Eq. (95) of Ref.<sup>16</sup>. Again, the off-diagonal entries of that matrix play the role of creation and annihilation operators, whose commutation relations are given in Eq. (98) of that reference. The latter commutation relations correspond to the usual Faddeev-Zamolodchikov algebra associated with the traditional ABCD form of the elements of the monodromy matrix. In turn, the above relations associated with the charge monodromy matrix refer to a different algebra. The corresponding form of that matrix was called ABCDF by the authors of Ref.<sup>16</sup>.

The main reason why the solution of the problem by the algebraic inverse scattering method<sup>16</sup> was achieved only thirty years after that of the coordinate Bethe ansatz<sup>15,17</sup> is that it was expected that the charge and spin monodromy matrices had the same traditional ABCD form<sup>24</sup>, consistently with the occurrence of a spin  $SU(2)$  symmetry and a charge (and  $\eta$ -spin)  $SU(2)$  symmetry known long ago<sup>55</sup>, associated with a global  $SO(4) = [SU(2) \times SU(2)]/Z_2$  symmetry<sup>10</sup>. Fortunately, the studies of Ref.<sup>16</sup> used an appropriate representation of the charge and spin monodromy matrices whose structure is able to distinguish creation and annihilation fields as well as possible *hidden symmetries*, as discussed by the authors of that reference.

A hidden symmetry beyond  $SO(4)$  was indeed identified recently: It is the charge global  $U(1)$  symmetry found in Ref.<sup>2</sup>. The studies of that reference reveal that for  $U/4t > 0$  the model charge and spin degrees of freedom are associated with  $U(2) = SU(2) \times U(1)$  and  $SU(2)$  symmetries, rather than with two  $SU(2)$  symmetries, respectively. The occurrence of such charge  $U(2) = SU(2) \times U(1)$  symmetry and spin  $SU(2)$  symmetry is fully consistent with the different ABCDF and ABCD forms of the charge and spin monodromy matrices of Eqs. (21) and (95) of Ref.<sup>16</sup>, respectively. Indeed, the former matrix is larger than the latter and involves more fields than expected from the global  $SO(4) = [SU(2) \times SU(2)]/Z_2$  symmetry alone, consistently with the global  $SO(3) \times SO(3) \times U(1) = [SO(4) \times U(1)]/Z_2$  symmetry of the model on the 1D and any other bipartite lattice<sup>2</sup>.

Our general description of the model on a square and 1D lattices takes such an extended global symmetry into account. Furthermore, for 1D it was also implicitly taken into account by the appropriate representation of the charge and spin monodromy matrices used in Ref.<sup>16</sup>. Such a consistency is a necessary condition for the  $c$  and  $\alpha\nu$  fermion operators emerging from the fields of the monodromy matrices upon diagonalization of the 1D problem for  $N_a \gg 1$ .

Initially the expressions obtained by the algebraic inverse scattering method for the Bethe states include both wanted terms and several types of unwanted terms. The latter terms are eliminated by imposing suitable restrictions to the rapidities. Such constraints lead to the Bethe-ansatz equations and ultimately to the real integer and half-integer quantum numbers, which in units of  $2\pi/L$  are the discrete momentum values that label the  $c$  and  $\alpha\nu$  fermion operators.

After solving the Bethe ansatz for both the charge and spin degrees of freedom, one reaches the charge rapidities  $\lambda_j$  with  $[N_a - 2S_\eta]$  values such that  $j = 1, \dots, [N_a - 2S_\eta]$  and the spin rapidities  $\tilde{\lambda}_j$  with  $[N_a/2 - S_\eta - S_s]$  values such that  $j = 1, \dots, [N_a/2 - S_\eta - S_s]$ . Here  $S_\eta = S_\eta^z$  and  $S_s = S_s^z$  for a HWS and  $S_\eta = -S_\eta^z$  and  $S_s = -S_s^z$  for a LWS of both the  $\eta$ -spin and spin algebras yet the rapidities can be extended to non-Bethe tower states provided that the number of their values are expressed in terms of  $S_\eta$  and  $S_s$  rather than of  $S_\eta^z$  and  $S_s^z$ , respectively. Equations of the same form as those obtained by the coordinate Bethe ansatz are reached by the algebraic operator formulation provided that one introduces the charge momentum rapidities  $k_j$  and spin rapidities  $\bar{\lambda}_j$  given by<sup>16</sup>  $z_-(\lambda_j) = [a(\lambda_j)/b(\lambda_j)] e^{2h(\lambda_j)} = e^{ik_j a}$  where  $j = 1, \dots, [N_a - 2S_\eta]$  and  $\bar{\lambda}_j = -i\tilde{\lambda}_j/2$  where  $j = 1, \dots, [N_a/2 - S_\eta - S_s]/2$ .

Before discussing the structure of the rapidities for  $N_a \gg 1$ , let us confirm that the numbers  $[N_a - 2S_\eta]$  and  $[N_a/2 - S_\eta - S_s]$  of discrete charge momentum and spin rapidity values, respectively, provided by the Bethe-ansatz solution are closely related to the occupancy configurations of the rotated electrons that are not invariant under the electron - rotated-electron unitary transformation. Indeed, such numbers can be rewritten as,

$$[N_a - 2S_\eta] = [2S_c + 2C_\eta]; \quad [N_a/2 - S_\eta - S_s] = [C_\eta + C_s], \quad (\text{B18})$$

where the numbers  $C_\eta$  and  $C_s$  are those of Eqs. (31), (47), and (51).

Here  $2S_c$  is the number of elementary rotated-electron charges associated with the singly occupied sites and  $2C_\eta = \sum_\nu 2\nu N_{\eta\nu}$  the number of such charges associated with the rotated-electron doubly occupied sites whose occupancy configurations are not invariant under the above unitary transformation. Moreover,  $[C_\eta + C_s] = \sum_{\alpha\nu} \nu N_{\alpha\nu}$  is the number  $C_\eta = \sum_\nu \nu N_{\eta\nu}$  of down spins (and up spins) of such rotated-electron doubly occupied sites plus the number  $C_s = \sum_\nu \nu N_{s\nu}$  of down spins (and up spins) of the rotated-electron singly occupied sites whose occupancy configurations are not invariant under that transformation.

The structure of the charge momentum and spin rapidities simplifies in the limit  $N_a \gg 1$ <sup>17</sup>. Then the  $[N_a - 2S_\eta] = [2S_c + 2C_\eta]$  charge momentum rapidity values separate into two classes corresponding to  $2S_c$  and  $2C_\eta$  of these values, respectively. The set of charge momentum rapidity values  $k_j$  such that  $j = 1, \dots, 2S_c$  are real and are related to the integer or half-integer quantum numbers  $I_j^c$  of Eq. (B14) such that  $q_j = [2\pi/L] I_j^c$  are the  $2S_c$  discrete momentum values occupied by the  $c$  fermions, out of a total number  $N_a$  of such values. That corresponds to the  $2S_c$  elementary charges of the rotated electrons that singly occupy sites.

Moreover, for  $N_a \gg 1$  the  $[N_a/2 - S_\eta - S_s] = [C_\eta + C_s]$  spin rapidity values separate into two classes corresponding to  $C_\eta$  and  $C_s$  of these values, respectively. The point is that the  $C_\eta$  down spins and  $C_\eta$  up spins of the rotated electrons that doubly occupy sites and whose occupancy configurations are not invariant under the electron - rotated-electron unitary transformation combine with the  $2C_\eta$  elementary charges left over by the above separation of the  $[N_a - 2S_\eta] = [2S_c + 2C_\eta]$  charge momentum rapidity values. Therefore,  $C_\eta$  spin rapidity values out of  $[C_\eta + C_s]$  combine with  $2C_\eta$  charge momentum rapidity values out of  $[2S_c + 2C_\eta]$ , leading to  $C_\eta$  new rapidity values associated with the  $\eta$ -spin singlet configurations. Those describe the  $\eta$ -spin degrees of freedom of the rotated electrons that doubly occupy sites and whose occupancy configurations are not invariant under the electron - rotated-electron unitary transformation.

In turn, the  $C_s$  spin rapidity values left over by the separation of the  $[N_a/2 - S_\eta - S_s] = [C_\eta + C_s]$  spin rapidity values describe the spin-singlet configurations associated with the rotated electrons that singly occupy sites and whose occupancy configurations are not invariant under the electron - rotated-electron unitary transformation. The charge degrees of freedom of these rotated electrons are described by the above set of charge momentum rapidity values  $k_j$  such that  $j = 1, \dots, 2S_c$ .

According to the  $N_a \gg 1$  results of Ref.<sup>17</sup>, the  $C_\eta$   $\eta$ -spin rapidity values (and  $C_s$  spin rapidity values) further separate into  $\eta\nu$  rapidities of length  $\nu = 1, 2, \dots$  with  $N_{\eta\nu}$  values (and  $s\nu$  rapidities of length  $\nu = 1, 2, \dots$  with  $N_{s\nu}$  values). Obviously, the sum-rules  $C_\eta = \sum_\nu \nu N_{\eta\nu}$  and  $C_s = \sum_\nu \nu N_{s\nu}$  are obeyed. The results of that reference reveal that  $s\nu$  rapidities of length  $\nu = 1$  are real and the imaginary part of the remaining branches of  $\alpha\nu$  rapidities where  $\alpha = \eta, s$  has a simple form.

Therefore, for  $N_a \gg 1$  the original Bethe-ansatz equations lead to a system of  $[1 + C_\eta + C_s]$  (infinite in the limit  $N_a \rightarrow \infty$ ) coupled thermodynamic equations whose solution gives the charge momentum rapidity values  $k_j$  such that  $j = 1, \dots, 2S_c$  and the values  $\Lambda_{j,\alpha\nu}$  of the real part of the  $\alpha\nu$  rapidities such that  $j = 1, \dots, N_{\alpha\nu}$  as a function of the occupancies of the real integer or half-integer quantum numbers  $I_j^c$  and  $I_j^{\alpha\nu}$  of Eq. (B14). Alike for the  $c$  fermions, the quantum numbers  $I_j^{\alpha\nu}$  such that  $q_j = [2\pi/L] I_j^{\alpha\nu}$  are the  $N_{\alpha\nu}$  discrete momentum values occupied by  $\alpha\nu$  fermions, out of a total number  $N_{\alpha\nu}$  of such values. (Note that here we used a notation suitable to our rotated-electron description of the problem and that in Ref.<sup>17</sup> such quantum numbers are denoted as in Eq. (B16) with  $\nu$  replaced by  $n$  and the values  $\Lambda_{j,\eta\nu}$  and  $\Lambda_{j,s\nu}$  of the real part of the rapidities by  $\Lambda_\alpha^n$  and  $\Lambda_\alpha^n$ , respectively, where  $\alpha$  plays the role of  $j$ .)

Summarizing the above discussion, in order to reach the  $c$  and  $\alpha\nu$  fermion operators the algebraic operator formulation of the diagonalization of the quantum problem starts by building up the Bethe states in terms of linear combination of products of the above mentioned several types of creation fields acting onto a suitable vacuum. The diagonalization of the charge and spin degrees of freedom involves the transfer matrices given in Eqs. (21) and (95) of Ref.<sup>16</sup>, respectively, whose off-diagonal entries are some of these creation and annihilation fields. The different form of such matrices is consistent with the model global  $SO(3) \times SO(3) \times U(1)$  symmetry, which is taken into account by our general description both for the model on the 1D and square lattices used in our studies of the square-lattice quantum liquid of  $c$  and  $s1$  fermions. The creation and annihilation fields obey the very involved commutation relations given in Eqs. (25), (40)-(42), (98), (B.1)-(B.3), (B.7)-(B.11), and (B.19)-(B.22) of Ref.<sup>16</sup> and are labeled by rapidities, which may be generally complex and are not the ultimate quantum numbers.

However, such creation and annihilation fields and their involved algebra generate expressions for the Bethe states that include both wanted terms and several types of unwanted and unphysical terms. Indeed, they act onto an extended and partially unphysical Hilbert space, larger than that of the model. The unwanted and unphysical terms are eliminated by imposing suitable restrictions to the rapidities that change the nature of the fields and for  $N_a \gg 1$  replace them by the  $c$  and  $\alpha\nu$  fermion operators labeled by the real integer and half-integer quantum numbers of the diagonalized model. Hence the Bethe-ansatz equations obtained by imposing suitable restrictions to the rapidities describe the relation between the rapidities and the ultimate quantum numbers associated with the  $c$  and  $\alpha\nu$  fermion operators.

In addition to emerging from the elimination of the unwanted and unphysical terms of the Bethe states generated by the initial creation and annihilation fields, the  $c$  and  $\alpha\nu$  fermion operator algebra refers to well-defined subspaces, which are spanned by energy eigenstates whose number of  $\eta$ -spinons, spinons, and  $c$  fermions is constant and given by  $N_{a_\eta} = [N_a - 2S_c]$ ,  $N_{a_s} = 2S_c$ , and  $N_c = 2S_c$ , respectively. Hence the number  $2S_c$  of rotated-electron singly occupied sites and the numbers  $N_{a_\eta}$  and  $N_{a_s}$  of sites of the  $\eta$ -spin and spin lattices, respectively, are constant.

As discussed in this paper, for both the model on 1D lattice considered in this Appendix and the model on the square lattice the  $S_c > 0$  vacuum of the LWS subspace  $|0_{\eta s}\rangle$  given in Eq. (23) is invariant under the electron - rotated-electron unitary transformation. For  $D = 1$  the  $N_{a_s}$  independent  $+1/2$  spinons of such a vacuum are the spins of  $N_{a_s}$  spin-up electrons, the  $N_{a_\eta}$  independent  $+1/2$   $\eta$ -spinons refer to the  $N_{a_\eta}$  sites unoccupied by electrons, and the  $N_c$   $c$  fermions describe the charge degrees of freedom of such electrons of the fully polarized state.

The corresponding LWSs that span the above subspace refer to rotated electrons rather than to electrons and have the general form given in Eq. (60) where the set of numbers  $\{N_{\alpha\nu}\}$  obey the sum-rule associated with the expressions given in Eq. (31), the  $\eta$ -spin ( $\alpha = \eta$ ) and spin ( $\alpha = s$ ) can have values  $S_\alpha = 0, \dots, N_{a_\alpha}/2$  such that  $S_\alpha = [N_{a_\alpha}/2 - C_\alpha]$ ,

and the set of numbers  $\{N_{a\nu}\}$  of discrete momentum values of each  $a\nu$  band are well defined and given by Eq. (42) and (43).

As mentioned previously, each subspace with constant values of  $S_c$  and hence also with constant values of  $N_{a\eta} = [N_a - 2S_c]$  and  $N_{a_s} = 2S_c$ , which the vacuum of Eq. (23) refers to, can be divided into smaller subspaces with constant values of  $S_c$ ,  $S_\eta$ , and  $S_s$  and hence also with constant values of  $C_\eta$  and  $C_s$ . Furthermore, the latter subspaces can be further divided into even smaller subspaces with constant values for the set of numbers  $\{N_{\eta\nu}\}$  and  $\{N_{s\nu}\}$ , which obey the sum-rule of Eq. (31).

Last but not least, since in contrast to the initial creation and annihilation fields the  $c$  and  $a\nu$  fermion operators generate the Bethe states free from unwanted and unphysical terms, are labeled by the quantum numbers of the diagonalized model, and their algebra does refer to the full LWS or HWS subspace but instead to subspaces spanned by well-defined types of Bethe states, there is no contradiction whatsoever between the charge ABCDF algebra<sup>16</sup> and spin ABCD traditional Faddeev-Zamolodchikov algebra<sup>24</sup> associated with involved commutation relations of the initial fields and the anticommutation relations of the  $c$  and  $a\nu$  fermion operators provided in Eqs. (B8) and (B9). Indeed, the initial creation and annihilation fields act onto an extended and partially unphysical Hilbert space whereas the  $c$  and  $a\nu$  fermion operators act onto well-defined subspaces of the model physical Hilbert space.

Upon acting onto such subspaces, the operators  $f_{q_j,c}^\dagger$  of the  $c$  fermions and  $f_{q_j,a\nu}^\dagger$  of the  $a\nu$  fermions have the expected simple anticommutation relations associated with those provided in Eqs. (B8) and (B9) for the corresponding operators  $f_{x_j,c}^\dagger$  and  $f_{x_j,a\nu}^\dagger$ , respectively. Moreover,  $c$  fermion operators commute with the  $a\nu$  fermion operators and  $a\nu$  and  $a'\nu'$  fermion operators belonging to different  $a\nu \neq a'\nu'$  branches also commute with each other.

Interestingly, in 1D our description may be used in the study of spectral functions involving matrix elements between Bethe states belonging to different subspaces with integer and half-integer character, respectively, for some of the quantum numbers of Eq. (B14). In that case the anticommutation relations of the operators  $f_{x_j,c}^\dagger$  and  $f_{x_j,a\nu}^\dagger$  remain as given in Eqs. (B8) and (B9) yet effective anticommutation relations, which take into account the shifts of the discrete momentum values upon the subspace transitions, must be used for the operators  $f_{q_j,c}^\dagger$  and  $f_{q_j,a\nu}^\dagger$ .

Finally, for the model on the 1D lattice in the one- and two-electron subspace as defined in this paper one may introduce a unitary transformation that under the ground-state - excited-state transitions, shifts the discrete momentum values  $q_j \rightarrow q_j + Q_c(q_j)/L$  of the  $c$  fermions and  $q_j \rightarrow q_j + Q_{s1}(q_j)/L$  of the  $s1$  fermions. Here  $Q_c(q_j)/2$  and  $Q_{s1}(q_j)/2$  are well-defined overall phase shifts generated by such transitions. That allows the evaluation for finite excitation energy of one- and two-electron matrix elements between the ground state and excited states and corresponding spectral-weight distributions for finite excitation energy  $\omega$ <sup>53</sup>. In the  $\omega \rightarrow 0$  limit that method provides the well known low-energy expressions predicted long ago by other techniques<sup>56</sup> and for finite  $\omega$  values successfully describes the unusual finite-energy one-electron spectral-weight distributions observed by photo-emission experiments in quasi-one-dimensional organic metals<sup>57</sup>.

Fortunately, the 1D dynamical theory of such papers refers to the one- and two-electron subspace where only the  $c$  and  $s1$  fermions have an active and explicit role. The anti-commuting algebra of the  $c$  and  $s1$  fermion operators and the expressions of Eqs. (8) and (24) apply to both the model in the square and 1D lattices and hence together with the consistency with the 1D exact solution found in this Appendix confirms the validity of the 1D dynamical theory. The general  $c$  and  $s1$  fermions considered here for the model on the square and 1D lattices correspond to the  $c$  and  $s1$  pseudoparticles of the 1D problem of Ref.<sup>53</sup>, respectively. In turn, the above shifted momentum values  $\tilde{q}_j \equiv q_j + Q_c(q_j)/L$  and  $\tilde{q}_j \equiv q_j + Q_{a\nu}(q_j)/L$  refer to the canonical momentum values of that reference and in its language label the  $c$  and  $s1$  pseudofermions, respectively, of the 1D *pseudofermion dynamical theory*.

### Appendix C: Subspace-dimension summation

In this Appendix we perform the subspace-dimension summation of Eq. (52) that runs over  $S_c$ ,  $S_\eta$ , and  $S_s$  integer and half-odd-integer values. Here we consider the square lattice so that  $D = 2$  in Eq. (52), yet the derivation proceeds in a similar way for  $D = 1$ . The subspace dimensions have the form  $d_r \cdot \prod_{\alpha=\eta,s} \mathcal{N}(S_\alpha, M_\alpha)$  given in Eq. (48) where  $d_r$  and  $\mathcal{N}(S_\alpha, M_\alpha)$  are provided in Eq. (49). Recounting the terms of Eq. (52), one may choose  $S_\eta$  to be the independent summation variable what gives,

$$\begin{aligned} & \sum_{S_c=0}^{N_a^2/2} \sum_{S_\eta=0}^{[N_a^2/2-S_c]} \sum_{S_s=0}^{S_c} \frac{1 + (-1)^{2(S_\eta+S_c)}}{2} \frac{1 + (-1)^{2(S_s+S_c)}}{2} \dots = \\ & = \sum_{S_\eta=0}^{N_a^2/2} \sum_{S_s=0}^{[N_a^2/2-S_\eta]} \sum_{S_c=S_s}^{[N_a^2/2-S_\eta]} \frac{1 + (-1)^{2(S_\eta+S_s)}}{2} \frac{1 + (-1)^{2(S_s+S_c)}}{2} \dots \end{aligned} \quad (C1)$$



One can then rewrite the summation (52) in the form,

$$\mathcal{N}_{tot} = \sum_{S_\eta=0}^{N_a^2/2} \sum_{S_s=0}^{[N_a^2/2-S_\eta]} \frac{1 + (-1)^{2(S_\eta+S_s)}}{2} (2S_\eta + 1)(2S_s + 1) \times \Sigma(S_\eta, S_s), \quad (C2)$$

where  $\Sigma(S_\eta, S_s)$  denotes the  $S_\eta$  and  $S_s$  dependent summation over  $S_c$  as follows,

$$\begin{aligned} \Sigma(S_\eta, S_s) = & \sum_{S_c=S_s}^{\frac{N_a^2}{2}-S_\eta} \frac{1 + (-1)^{2(S_s+S_c)}}{2} \binom{N_a^2}{2S_c} \times \\ & \left[ \binom{N_a^2 - 2S_c}{\frac{N_a^2}{2} - S_c - S_\eta} - \binom{N_a^2 - 2S_c}{\frac{N_a^2}{2} - S_c - S_\eta - 1} \right] \left[ \binom{2S_c}{S_c - S_s} - \binom{2S_c}{S_c - S_s - 1} \right] \\ & \sum_{S_c=S_s}^{\frac{N_a^2}{2}-S_\eta} \frac{1 + (-1)^{2(S_s+S_c)}}{2} N_a^2! \left[ \frac{1}{(S_c - S_s)!(S_c + S_s)!} - \frac{1}{(S_c - S_s - 1)!(S_c + S_s + 1)!} \right] \times \\ & \left[ \frac{1}{(N_a^2/2 - S_c - S_\eta)!(N_a^2/2 - S_c + S_\eta)!} - \frac{1}{(N_a^2/2 - S_c - S_\eta - 1)!(N_a^2/2 - S_c + S_\eta + 1)!} \right]. \quad (C3) \end{aligned}$$

In order to evaluate  $\Sigma(S_\eta, S_s)$  it is useful to replace the variable  $S_c$  by  $k = S_c - S_s$ . To simplify the notation we then introduce,

$$\mathcal{S} = S_\eta + S_s = \mathcal{S}(S_\eta, S_s); \quad \mathcal{D} = S_\eta - S_s = \mathcal{D}(S_\eta, S_s). \quad (C4)$$

Due to the parity factor, in the summation over  $k$  only the terms with  $k$  integer survive so that,

$$\begin{aligned} \Sigma = & \sum_{k=0}^{\frac{N_a^2}{2}-\mathcal{S}} N_a^2! \left[ \frac{1}{k! (\mathcal{S} - \mathcal{D} + k)!} - \frac{1}{(k-1)! (\mathcal{S} - \mathcal{D} + k + 1)!} \right] \times \\ & \left[ \frac{1}{(N_a^2/2 - \mathcal{S} - k)! (N_a^2/2 + \mathcal{D} - k)!} - \frac{1}{(N_a^2/2 - \mathcal{S} - k - 1)! (N_a^2/2 + \mathcal{D} - k + 1)!} \right] \\ = & \sum_{k=0}^{\frac{N_a^2}{2}-\mathcal{S}} N_a^2! \left\{ \frac{1}{k! (\mathcal{S} - \mathcal{D} + k)!} \frac{1}{(N_a^2/2 - \mathcal{S} - k)! (N_a^2/2 + \mathcal{D} - k)!} - \right. \\ & - \frac{1}{k! (\mathcal{S} - \mathcal{D} + k)!} \frac{1}{(N_a^2/2 - \mathcal{S} - k - 1)! (N_a^2/2 + \mathcal{D} - k + 1)!} - \\ & - \frac{1}{(k-1)! (\mathcal{S} - \mathcal{D} + k + 1)!} \frac{1}{(N_a^2/2 - \mathcal{S} - k)! (N_a^2/2 + \mathcal{D} - k)!} + \\ & \left. + \frac{1}{(k-1)! (\mathcal{S} - \mathcal{D} + k + 1)!} \frac{1}{(N_a^2/2 - \mathcal{S} - k - 1)! (N_a^2/2 + \mathcal{D} - k + 1)!} \right\}, \quad (C5) \end{aligned}$$

where now the  $k$  summation runs over integers only.

In order to perform the summation (C5) we rearrange the terms as follows,

$$\begin{aligned} \Sigma = & \sum_{k=0}^{\frac{N_a^2}{2}-\mathcal{S}} \left\{ \frac{1}{(N_a^2/2 + \mathcal{D})! (N_a^2/2 - \mathcal{D})!} \left[ \binom{N_a^2/2 + \mathcal{D}}{k} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - k} + \binom{N_a^2/2 + \mathcal{D}}{k-1} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - k - 1} \right] - \right. \\ & - \frac{1}{(N_a^2/2 + \mathcal{D} + 1)! (N_a^2/2 - \mathcal{D} - 1)!} \binom{N_a^2/2 + \mathcal{D} + 1}{k} \binom{N_a^2/2 - \mathcal{D} - 1}{N_a^2/2 - \mathcal{S} - k - 1} - \\ & \left. - \frac{1}{(N_a^2/2 + \mathcal{D} - 1)! (N_a^2/2 - \mathcal{D} + 1)!} \binom{N_a^2/2 + \mathcal{D} - 1}{k-1} \binom{N_a^2/2 - \mathcal{D} + 1}{N_a^2/2 - \mathcal{S} - k} \right\} N_a^2!, \quad (C6) \end{aligned}$$

or

$$\begin{aligned}
\Sigma = & \binom{N_a^2}{N_a^2/2 - \mathcal{D}} \sum_{k=0}^{\frac{N_a^2}{2} - \mathcal{S}} \left[ \binom{N_a^2/2 + \mathcal{D}}{k} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - k} + \binom{N_a^2/2 + \mathcal{D}}{k-1} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - k - 1} \right] - \\
& - \binom{N_a^2}{N_a^2/2 - \mathcal{D} - 1} \sum_{k=0}^{\frac{N_a^2}{2} - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D} + 1}{k} \binom{N_a^2/2 - \mathcal{D} - 1}{N_a^2/2 - \mathcal{S} - k - 1} - \\
& - \binom{N_a^2}{N_a^2/2 - \mathcal{D} + 1} \sum_{k=0}^{\frac{N_a^2}{2} - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D} - 1}{k-1} \binom{N_a^2/2 - \mathcal{D} + 1}{N_a^2/2 - \mathcal{S} - k}.
\end{aligned} \tag{C7}$$

Next, by using the identity,

$$\sum_{k=0}^N \binom{A}{k} \binom{B}{N-k} = \binom{A+B}{N}, \tag{C8}$$

we carry out separately the summations in expression (C7), what gives,

$$\sum_{k=0}^{N_a^2/2 - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D}}{k} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - k} = \binom{N_a^2}{N_a^2/2 - \mathcal{S}}, \tag{C9}$$

$$\begin{aligned}
\sum_{k=0}^{N_a^2/2 - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D}}{k-1} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - k - 1} &= \sum_{k=1}^{N_a^2/2 - \mathcal{S} - 1} \binom{N_a^2/2 + \mathcal{D}}{k-1} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - k - 1} \\
&= \sum_{k'=0}^{N_a^2/2 - \mathcal{S} - 2} \binom{N_a^2/2 + \mathcal{D}}{k'} \binom{N_a^2/2 - \mathcal{D}}{N_a^2/2 - \mathcal{S} - 2 - k'} \\
&= \binom{N_a^2}{N_a^2/2 - \mathcal{S} - 2},
\end{aligned} \tag{C10}$$

$$\begin{aligned}
\sum_{k=0}^{N_a^2/2 - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D} + 1}{k} \binom{N_a^2/2 - \mathcal{D} - 1}{N_a^2/2 - \mathcal{S} - k - 1} &= \sum_{k=0}^{N_a^2/2 - \mathcal{S} - 1} \binom{N_a^2/2 + \mathcal{D} + 1}{k} \binom{N_a^2/2 - \mathcal{D} - 1}{N_a^2/2 - \mathcal{S} - 1 - k} \\
&= \binom{N_a^2}{N_a^2/2 - \mathcal{S} - 1},
\end{aligned} \tag{C11}$$

and

$$\begin{aligned}
\sum_{k=0}^{N_a^2/2 - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D} - 1}{k-1} \binom{N_a^2/2 - \mathcal{D} + 1}{N_a^2/2 - \mathcal{S} - k} &= \sum_{k=1}^{N_a^2/2 - \mathcal{S}} \binom{N_a^2/2 + \mathcal{D} - 1}{k-1} \binom{N_a^2/2 - \mathcal{D} + 1}{N_a^2/2 - \mathcal{S} - k} \\
&= \sum_{k'=0}^{N_a^2/2 - \mathcal{S} - 1} \binom{N_a^2/2 + \mathcal{D} - 1}{k'} \binom{N_a^2/2 - \mathcal{D} + 1}{N_a^2/2 - \mathcal{S} - 1 - k'} \\
&= \binom{N_a^2}{N_a^2/2 - \mathcal{S} - 1}.
\end{aligned} \tag{C12}$$

Introducing these results in expression (C7) for  $\Sigma$  leads to,

$$\begin{aligned}
\Sigma(S_\eta, S_s) &= \binom{N_a^2}{N_a^2/2 - \mathcal{D}} \left[ \binom{N_a^2}{N_a^2/2 - \mathcal{S}} + \binom{N_a^2}{N_a^2/2 - \mathcal{S} - 2} \right] - \\
&\quad - \binom{N_a^2}{N_a^2/2 - \mathcal{S} - 1} \left[ \binom{N_a^2}{N_a^2/2 - \mathcal{D} + 1} + \binom{N_a^2}{N_a^2/2 - \mathcal{D} - 1} \right] \\
&\equiv \Sigma(\mathcal{S}, \mathcal{D}).
\end{aligned} \tag{C13}$$

Expression (C2) for  $\mathcal{N}_{tot}$  can now be rewritten as,

$$\begin{aligned} \mathcal{N}_{tot} = & \sum_{S_\eta=0}^{N_a^2/2} \sum_{S_s=0}^{[N_a^2/2-S_\eta]} \frac{1+(-1)^{2(S_\eta+S_s)}}{2} (2S_\eta+1)(2S_s+1) \times \\ & \left\{ \binom{N_a^2}{N_a^2/2-(S_\eta-S_s)} \left[ \binom{N_a^2}{N_a^2/2-(S_\eta+S_s)} + \binom{N_a^2}{N_a^2/2-(S_\eta+S_s)-2} \right] - \right. \\ & \left. - \binom{N_a^2}{N_a^2/2-(S_\eta+S_s)-1} \left[ \binom{N_a^2}{N_a^2/2-(S_\eta-S_s)+1} + \binom{N_a^2}{N_a^2/2-(S_\eta-S_s)-1} \right] \right\}, \end{aligned} \quad (C14)$$

where the summations run over both integers and half-odd integers. The use of the notation (C4) then allows rewriting (C14) in compact form,

$$\mathcal{N}_{tot} = \sum_{S_\eta=0}^{N_a^2/2} \sum_{S_s=0}^{[N_a^2/2-S_\eta]} \frac{1+(-1)^{2S}}{2} (S+\mathcal{D}+1)(S-\mathcal{D}+1) \times \Sigma(S, \mathcal{D}), \quad (C15)$$

where the summations run again over both integers and half-odd integers.

We can perform the summations of Eq. (C15) in the integers  $\mathcal{S}$  and  $\mathcal{D}$  instead of in  $S_\eta$  and  $S_s$ . Indeed, the first factor cancels all the terms with  $\mathcal{S}$  and  $\mathcal{D}$  non-integer so that,

$$\begin{aligned} \sum_{S_\eta=0}^{N_a^2/2} \sum_{S_s=0}^{[N_a^2/2-S_\eta]} \frac{1+(-1)^{2(S_\eta+S_s)}}{2} \cdots (S_\eta \text{ and } S_s \text{ both either integers or half odd integers}) = \\ = \sum_{S=0}^{N_a^2/2} \sum_{\mathcal{D}=-S}^{+\mathcal{S}} \cdots (\mathcal{S} \text{ and } \mathcal{D} \text{ integers}). \end{aligned}$$

Thus we find,

$$\mathcal{N}_{tot} = \sum_{S=0}^{N_a^2/2} \sum_{\mathcal{D}=-S}^{+\mathcal{S}} ((S+1)^2 - \mathcal{D}^2) \times \Sigma(\mathcal{S}, \mathcal{D}).$$

The use of the result (C13) then leads to,

$$\begin{aligned} \mathcal{N}_{tot} = \sum_{S=0}^{N_a^2/2} \sum_{\mathcal{D}=-S}^{+\mathcal{S}} ((S+1)^2 - \mathcal{D}^2) \left\{ \binom{N_a^2}{N_a^2/2-\mathcal{D}} \left[ \binom{N_a^2}{N_a^2/2-\mathcal{S}} + \binom{N_a^2}{N_a^2/2-\mathcal{S}-2} \right] - \right. \\ \left. - \binom{N_a^2}{N_a^2/2-\mathcal{S}-1} \left[ \binom{N_a^2}{N_a^2/2-\mathcal{D}+1} + \binom{N_a^2}{N_a^2/2-\mathcal{D}-1} \right] \right\}. \end{aligned} \quad (C16)$$

Replacing the variable  $\mathcal{S}$  by  $\mathcal{S}' = \mathcal{S} + 1$  we reach a more tractable expression for  $\mathcal{N}_{tot}$ ,

$$\mathcal{N}_{tot} = \sum_{S'=1}^{N_a^2/2+1} \sum_{\mathcal{D}=-S'+1}^{S'-1} \mathcal{T}(S', \mathcal{D}), \quad (C17)$$

where

$$\begin{aligned} \mathcal{T}(S', \mathcal{D}) &= ((S')^2 - \mathcal{D}^2) \times \Sigma(S' - 1, \mathcal{D}) \\ &= (S'^2 - \mathcal{D}^2) \left\{ \binom{N_a^2}{N_a^2/2-\mathcal{D}} \left[ \binom{N_a^2}{N_a^2/2-S'+1} + \binom{N_a^2}{N_a^2/2-S'-1} \right] - \right. \\ &\quad \left. - \binom{N_a^2}{N_a^2/2-S'} \left[ \binom{N_a^2}{N_a^2/2-\mathcal{D}+1} + \binom{N_a^2}{N_a^2/2-\mathcal{D}-1} \right] \right\}, \end{aligned} \quad (C18)$$

is completely symmetric in the summation variables.

Since  $\mathcal{T}(\mathcal{S}', \mathcal{D} = \pm \mathcal{S}') = 0$ , we can extend the summation over  $\mathcal{D}$  of Eq.(C17) to  $\mathcal{D} = \pm \mathcal{S}'$ . We then formally extend the summation over  $\mathcal{S}'$  to  $\mathcal{S}' = 0$  because the corresponding term vanishes:  $\mathcal{T}(\mathcal{S}' = 0, \mathcal{D} = 0) = 0$ . Furthermore,  $\mathcal{T}(\pm \mathcal{S}', \mathcal{D}) = \mathcal{T}(\mathcal{S}', \pm \mathcal{D}) = \mathcal{T}(\mathcal{S}', \mathcal{D})$ , and due to the symmetry  $\mathcal{S}' \leftrightarrow \mathcal{D}$  we can write,

$$\sum_{\mathcal{S}'=1}^{N_a^2/2} \sum_{\mathcal{D}=-\mathcal{S}'+1}^{\mathcal{S}'-1} \mathcal{T}(\mathcal{S}', \mathcal{D}) = \frac{1}{4} \sum_{\mathcal{S}', \mathcal{D}=-(N_a^2/2+1)}^{N_a^2/2+1} \mathcal{T}(\mathcal{S}', \mathcal{D}). \quad (\text{C19})$$

Let us introduce the numbers  $p$  and  $q$  such that,

$$\begin{aligned} \mathcal{S}' + N_a^2/2 + 1 &= p \Leftrightarrow \mathcal{S}' = p - (N_a^2/2 + 1) \\ \mathcal{D} + N_a^2/2 + 1 &= q \Leftrightarrow \mathcal{D} = q - (N_a^2/2 + 1). \end{aligned}$$

The use of (C19) then allows rewriting (C17) as,

$$\begin{aligned} \mathcal{N}_{tot} &= \frac{1}{4} \sum_{p,q=0}^{N_a^2+2} [q(N_a^2 + 2 - q) - p(N_a^2 + 2 - p)] \\ &\quad \times \left\{ \binom{N_a^2}{q-1} \left[ \binom{N_a^2}{p} + \binom{N_a^2}{p-2} \right] - \binom{N_a^2}{p-1} \left[ \binom{N_a^2}{q} + \binom{N_a^2}{q-2} \right] \right\}. \end{aligned} \quad (\text{C20})$$

This expression can be simplified noticing that,

$$\binom{N}{x} + \binom{N}{x-2} = -2 \binom{N}{x-1} + \binom{N+2}{x}.$$

Replacing in Eq.(C20) one then finds,

$$\begin{aligned} \mathcal{N}_{tot} &= \frac{1}{4} \sum_{p,q=0}^{N_a^2+2} \left[ q(N_a^2 + 2 - q) - p(N_a^2 + 2 - p) \right] \left\{ \binom{N_a^2}{q-1} \binom{N_a^2+2}{p} - \binom{N_a^2}{p-1} \binom{N_a^2+2}{q} \right\} \\ &= \frac{1}{4} \sum_{p,q=0}^{N_a^2+2} \left\{ q(N_a^2 + 2 - q) \left[ \binom{N_a^2}{q-1} \binom{N_a^2+2}{p} - \binom{N_a^2}{p-1} \binom{N_a^2+2}{q} \right] + (q \leftrightarrow p) \right\} \\ &= \frac{1}{4} 2 \left\{ \sum_{q=0}^{N_a^2+2} q(N_a^2 + 2 - q) \binom{N_a^2}{q-1} \sum_{p=0}^{N_a^2+2} \binom{N_a^2+2}{p} - \sum_{q=0}^{N_a^2+2} q(N_a^2 + 2 - q) \binom{N_a^2+2}{q} \sum_{p=0}^{N_a^2+2} \binom{N_a^2}{p-1} \right\}. \end{aligned} \quad (\text{C21})$$

Finally, the use of the identities,

$$\begin{aligned} \sum_{k=0}^N \binom{N}{k} &= 2^N, \\ \sum_{k=0}^{N+2} \binom{N}{k-1} &= \sum_{k=1}^{N+1} \binom{N}{k-1} = \sum_{k'=0}^N \binom{N}{k'} = 2^N, \\ \sum_{k=0}^N k(N-k) \binom{N}{k} &= \sum_{k=1}^{N-1} \frac{N!}{(k-1)!(N-k-1)!} = N(N-1) \sum_{k=1}^{N-2} \binom{N-2}{k-1} \\ &= N(N-1) 2^{N-2}, \end{aligned}$$

and

$$\begin{aligned} \sum_{k=0}^{N+2} k(N+2-k) \binom{N}{k-1} &= \sum_{k=1}^{N+1} k(N+2-k) \binom{N}{k-1} = \sum_{k=1}^N k(N+2-k) \binom{N}{k-1} \\ &= \sum_{k'=0}^N (k'+1)(N-k'+1) \binom{N}{k'} = \sum_{k'=0}^N [k'(N-k') + (N+1)] \binom{N}{k'} \\ &= N(N-1) 2^{N-2} + (N+1) 2^N = 2^{N-2} [N(N-1) + 4(N+1)] \\ &= [N^2 + 3N + 4] 2^{N-2}, \end{aligned}$$

leads to,

$$\mathcal{N}_{tot} = \frac{1}{2} \left\{ [N_a^2 + 3N_a^2 + 4] 2^{N_a^2-2} \times 2^{N_a^2+2} - (N_a^2 + 2)(N_a^2 + 1) 2^{N_a^2} \times 2^{N_a^2} \right\} = \frac{1}{2} 2^{2N_a^2} \times 2 = 4^{N_a^2}, \quad (\text{C22})$$

which is the desired result.

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